Generalised Interaction Mining: Probabilistic, Statistical and Vectorised Methods in High Dimensional or Uncertain Databases

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für Brigitte, Martin, Mundi & Michael

Abstract

Knowledge Discovery in Databases (KDD) is the non-trivial process of identifying valid, novel, useful and ultimately understandable patterns in data. The core step of the KDD process is the application of Data Mining (DM) algorithms to efficiently find interesting patterns in large databases. This thesis concerns itself with three inter-related themes: Generalised interaction and rule mining; the incorporation of statistics into novel data mining approaches; and probabilistic frequent pattern mining in uncertain databases.

An interaction describes an effect that variables have – or appear to have – on each other. Interaction mining is the process of mining structures on variables describing their interaction patterns – usually represented as sets, graphs or rules. Interactions may be complex, represent both positive and negative relationships, and the presence of interactions can influence another interaction or variable in interesting ways. Finding interactions is useful in domains ranging from social network analysis, marketing, the sciences, e-commerce, to statistics and finance. Many data mining tasks may be considered as mining interactions, such as clustering; frequent itemset mining; association rule mining; classification rules; graph mining; flock mining; etc. Interaction mining problems can have very different semantics, pattern definitions, interestingness measures and data types. Solving a wide range of interaction mining problems at the abstract level, and doing so efficiently – ideally more efficiently than with specialised approaches, is a challenging problem.

This thesis introduces and solves the Generalised Interaction Mining (GIM) and Generalised Rule Mining (GRM) problems. GIM and GRM use an efficient and intuitive computational model based purely on vector valued functions. The semantics of the interactions, their interestingness measures and the type of data considered are flexible components of vectorised frameworks. By separating the semantics of a problem from the algorithm used to mine it, the frameworks allow both to vary independently of each other. This makes it easier to develop new methods by focusing purely on a problem's semantics and removing the burden of designing an

efficient algorithm. By encoding interactions as vectors in the space (or a sub-space) of samples, they provide an intuitive geometric interpretation that inspires novel methods. By operating in time linear in the number of interesting interactions that need to be examined, the GIM and GRM algorithms are optimal. The use of GRM or GIM provides efficient solutions to a range of problems in this thesis, including graph mining, counting based methods, itemset mining, clique mining, a clustering problem, complex pattern mining, negative pattern mining, solving an optimisation problem, spatial data mining, probabilistic itemset mining, probabilistic association rule mining, feature selection and generation, classification and multiplication rule mining.

Data mining is a hypothesis generating endeavour, examining large databases for patterns suggesting novel and useful knowledge to the user. Since the database is a sample, the patterns found should describe hypotheses about the underlying process generating the data. In searching for these patterns, a DM algorithm makes additional hypothesis when it prunes the search space. Natural questions to ask then, are: "Does the algorithm find patterns that are statistically significant?" and "Did the algorithm make significant decisions during its search?". Such questions address the quality of patterns found though data mining and the confidence that a user can have in utilising them. Finally, statistics has a range of useful tools and measures that are applicable in data mining. In this context, this thesis incorporates statistical techniques – in particular, non-parametric significance tests and correlation – directly into novel data mining approaches. This idea is applied to statistically significant and relatively class correlated rule based classification of imbalanced data sets; significant frequent itemset mining; mining complex correlation structures between variables for feature selection; mining correlated multiplication rules for interaction mining and feature generation; and conjunctive correlation rules for classification. The application of GIM or GRM to these problems lead to efficient and intuitive solutions.

Frequent itemset mining (FIM) is a fundamental problem in data mining. While it is usually assumed that the items occurring in a transaction are known for certain, in many applications the data is inherently noisy or probabilistic; such as adding noise in privacy preserving data mining applications, aggregation or grouping of records leading to estimated purchase probabilities, and databases capturing naturally uncertain phenomena. The consideration of existential uncertainty of item(sets) makes traditional techniques inapplicable. Prior to the work in this thesis, itemsets were mined if their expected support is high. This returns only an estimate, ignores the probability distribution of support, provides no confidence in the results, and can

lead to scenarios where itemsets are labeled frequent even if they are more likely to be infrequent. Clearly, this is undesirable. This thesis proposes and solves the Probabilistic Frequent Itemset Mining (PFIM) problem, where itemsets are considered interesting if the *probability* that they are frequent is high. The problem is solved under the possible worlds model and a proposed probabilistic framework for PFIM. Novel and efficient methods are developed for computing an itemset's exact support probability distribution and frequentness probability, using the Poisson binomial recurrence, generating functions, or a Normal approximation. Incremental methods are proposed to answer queries such as finding the top-k probabilistic frequent itemsets. A number of specialised PFIM algorithms are developed, with each being more efficient than the last: ProApriori is the first solution to PFIM and is based on candidate generation and testing. ProFP-Growth is the first probabilistic FP-Growth type algorithm and uses a proposed probabilistic frequent pattern tree (Pro-FPTree) to avoid candidate generation. Finally, the application of GIM leads to GIM-PFIM; the fastest known algorithm for solving the PFIM problem. It achieves orders of magnitude improvements in space and time usage, and leads to an intuitive subspace and probability-vector based interpretation of PFIM.

Zusammenfassung

Knowledge Discovery in Datenbanken (KDD) ist der nicht-triviale Prozess, gültiges, neues, potentiell nützliches und letztendlich verständliches Wissen aus großen Datensätzen zu extrahieren. Der wichtigste Schritt im KDD Prozess ist die Anwendung effizienter Data Mining (DM) Algorithmen um interessante Muster ("Patterns") in Datensätzen zu finden. Diese Dissertation beschäftigt sich mit drei verwandten Themen: Generalised Interaction und Rule Mining, die Einbindung von statistischen Methoden in neue DM Algorithmen und Probabilistic Frequent Itemset Mining (PFIM) in unsicheren Daten.

Eine Interaktion ("Interaction") beschreibt den Einfluss, den Variablen aufeinander haben. Interaktionsmining ist der Prozess, Strukturen zwischen Variablen zu finden, die Interaktionsmuster beschreiben. Diese werden gewöhnlicherweise als Mengen, Graphen oder Regeln repräsentiert. Interaktionen können komplex sein und sowohl positive als auch negative Beziehungen repräsentieren. Außerdem kann das Vorhandensein von Interaktionen andere Interaktionen oder Variablen beeinflussen. Interaktionen stellen in Bereichen wie Soziale Netzwerk Analyse, Marketing, Wissenschaft, E-commerce, Statistik und Finanz wertvolle Information dar. Viele DM Methoden können als Interaktionsmining betrachtet werden: Zum Beispiel Clustering, Frequent Itemset Mining, Assoziationsregeln, Klassifikationsregeln, Graph Mining, Flock Mining, usw. Interaktionsmining-Probleme können sehr unterschiedliche Semantik, Musterdefinitionen, Interessantheitsmaße und Datentypen erfordern. Interaktionsmining-Probleme auf breiter und abstrakter Basis effizient – und im Idealfall effizienter als mit spezialisierten Methoden – zu lösen, ist ein herausforderndes Problem.

Diese Dissertation führt das Generalised Interaction Mining (GIM) und das Generalised Rule Mining (GRM) Problem ein und beschreibt Lösungen für diese. GIM und GRM benutzen ein effizientes und intuitives Berechnungsmodell, das einzig und allein auf vektorbasierten Funktionen beruht. Die Semantik der Interaktionen, ihre Interessantheitsmaße und die Datenarten, sind Komponenten in vektorisierten Frameworks. Die Frameworks ermöglichen die Trennung der Problemsemantik vom

Algorithmus, so dass beide unabhängig voneinander geändert werden können. Die Entwicklung neuer Methoden wird dadurch erleichtert, da man sich völlig auf die Problemsemantik fokussieren kann und sich nicht mit der Entwicklung problemspezifischer Algorithmen befassen muss. Die Kodierung der Interaktionen als Vektoren im gesamten Raum (oder Teilraum) der Stichproben stellt eine intuitive geometrische Interpretation dar, die neuartige Methoden inspiriert. Die GRM- und GIM- Algorithmen haben lineare Laufzeit in der Anzahl der Interaktionen die geprüft werden müssen und sind somit optimal. Die Anwendung von GRM oder GIM in dieser Dissertation ermöglicht effiziente Lösungen für eine Reihe von Problemen, wie zum Beispiel Graph Mining, Aufzählungsmethoden, Itemset Mining, Clique Mining, ein Clusteringproblem, das Finden von komplexen und negativen Mustern, die Lösung von Optimierungsproblemen, Spatial Data Mining, probabilistisches Itemset Mining, probabilistisches Mining von Assoziationsregel, Selektion und Erzeugung von Features, Mining von Klassifikations- und Multiplikationsregel, u.v.m.

Data Mining ist ein Verfahren, das Hypothesen produziert, indem es in großen Datensätzen Muster findet und damit für den Anwender neues und nützliches Wissen vorschlägt. Da die untersuchte Datenbank ein Resultat des datenerzeugenden Prozesses ist, sollten die gefundenen Muster Erkenntnisse über diesen Prozess liefern. Bei der Suche nach diesen Mustern macht ein DM Algorithmus zusätzliche Hypothesen, wenn Teile des Suchraums ausgeschlossen werden. Die folgenden Fragen sind dabei wichtig: “Findet der Algorithmus statistisch signifikante Muster?” und “Hat der Algorithmus während des Suchprozesses signifikante Entscheidungen getroffen?”. Diese Fragen beeinflussen die Qualität der Muster und die Sicherheit die der Anwender in ihrer Benutzung haben kann. Da die Statistik auch eine Reihe von nützlichen Methoden bereitstellt, die für DM anwendbar sind, kombiniert diese Dissertation einige statistische Methoden mit neuen DM Algorithmen, insbesondere nicht-parametrische Signifikanztests und Korrelation. Diese Idee wird für die folgenden Probleme angewandt: Signifikante und "relatively class correlated" regelbasierte Klassifikation in unsymmetrischen Datensätzen, signifikantes Frequent Itemset Mining, Mining von komplizierten Korrelationsstrukturen zwischen Variablen zum Zweck der Featureselektion, Mining von korrelierten Multiplikationsregeln zum Zwecke des Interaktionsminings und Featureerzeugung und konjunktive Korrelationsregeln für die Klassifikation. Die Anwendung von GIM und GRM auf diese Probleme führt zu effizienten und intuitiven Lösungen.

Frequent Itemset Mining (FIM) ist ein fundamentales Problem im Data Mining. Obwohl allgemein die Annahme gilt, dass in einer Transaktion enthaltene Items bekannt sind, sind die Daten in vielen Anwendungen unsicher oder probabilistisch.

Beispiele sind das Hinzufügen von Rauschen zu Datenschutzzwecken, die Gruppierung von Datensätzen die zu geschätzten Kaufwahrscheinlichkeiten führen und Datensätze deren Herkunft von Natur aus unsicher sind. Die Berücksichtigung von unsicheren Datensätzen verhindert die Anwendung von traditionellen Methoden. Vor der Arbeit in dieser Dissertation wurden Itemsets gesucht, deren erwartetes Vorkommen hoch ist. Diese Methode produziert jedoch nur Schätzwerte, vernachlässigt die Wahrscheinlichkeitsverteilung der Vorkommen, bietet keine Sicherheit für die Genauigkeit der Ergebnisse und kann zu Szenarien führen in denen das Vorkommen als häufig eingestuft wird, obwohl die Wahrscheinlichkeit höher ist, dass sie nur selten vorkommen. Solche Ergebnisse sind natürlich unerwünscht. Diese Dissertation führt das Probabilistic Frequent Itemset Mining (PFIM) ein. Diese Lösung betrachtet Itemsets als interessant, wenn die Wahrscheinlichkeit groß ist, dass sie häufig vorkommen. Die Problemlösung besteht aus der Anwendung des Possible Worlds Models und dem vorgeschlagenen probabilistisches Framework für PFIM. Es werden neue und effiziente Methoden entwickelt um die Wahrscheinlichkeitsverteilung des Vorkommens und die Häufigkeitsverteilung eines Itemsets zu berechnen. Dazu werden die Poisson Binomial Recurrence, Generating Functions, oder eine normalverteilte Annäherung verwendet. Inkrementelle Methoden werden vorgeschlagen um Fragen wie "Finde die top-k Probabilistic Frequent Itemsets" zu beantworten. Mehrere PFIM Algorithmen werden entwickelt, wobei die Effizienz von Algorithmus zu Algorithmus steigt: ProApriori ist die erste Lösung für PFIM und basiert auf erzeugen und testen von Kandidaten. ProFP-Growth ist der erste probabilistische FP-Growth Algorithmus. Er schlägt einen Probabilistic Frequent Pattern Tree (Pro-FPTree) vor, der Kandidatenerzeugung überflüssig macht. Die Anwendung von GIM führt schließlich zu GIM-PFIM, dem schnellsten bekannten Algorithmus zur Lösung des PFIM Problems. Dieser Algorithmus resultiert in einem um Größenordnungen besseren Zeit- und Speicherbedarf, und führt zu einer intuitiven Interpretation von PFIM, basierend auf Unterräumen und Wahrscheinlichkeitsvektoren.

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Last but definitely not least, I am very grateful for the support of my family – and in particular my parents for their never ending encouragement.

Publications

Publications during the author's Doctoral and PhD candidatures are listed below. [18] and [19] were joint work with the team in Professor Hans-Peter Kriegel's database systems group in the Ludwig-Maximilians-Universität, Munich, Germany. [94] was joint work with Ghazi Al-Naymat at the University of Sydney.

Publications Contributing to this Thesis

The following publications contributed to this thesis, as will be described in section 1.2.

- [19] Thomas Bernecker, Hans-Peter Kriegel, Matthias Renz, Florian Verhein, Andreas Züfle: *Probabilistic Frequent Pattern Growth for Itemset Mining in Uncertain Databases*
  Technical report, arXiv.org, arXiv:1008.2300v1, Fri, 13 Aug 2010.

- [93] Florian Verhein: *Generalised Rule Mining*
  The 15th International Conference on Database Systems for Advanced Applications (DASFAA'2010), 1 – 4 April 2010, Tsukuba, Japan. Lecture Notes in Computer Science, Volume 5981/2010, pp. 85-92, Springer, 2010.

- [18] Thomas Bernecker, Hans-Peter Kriegel, Matthias Renz, Florian Verhein, Andreas Züfle: *Probabilistic Frequent Itemset Mining in Uncertain Databases*
  The 15th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (SIGKDD'2009). Paris, France, June 28 – July 1 2009. pp. 119-128, ACM Press, 2009.

- [91] Florian Verhein: *Mining Complete Complex Maximal Sets of Correlated Variables with Applications to Feature Subset Selection*
  2008 SIAM International Conference on Data Mining (SDM'2008). April 24-26 2008, Atlanta, Georgia, USA. pp. 597-608, SIAM, 2008.

- [94] Florian Verhein, Ghazi Al-Naymat: *Fast Mining of Complex Spatial Co-location Patterns using GLIMIT*
  IEEE International Conference on Data Mining Workshops (ICDM-W'2007). 28 – 31 October 2007, Omaha NE, USA. pp. 679-684, IEEE Computer Society, 2007.

- [98] Florian Verhein, Sanjay Chawla: *Using Significant, Positively Associated and Relatively Class Correlated Rules For Associative Classification of Imbalanced Datasets*
  IEEE International Conference on Data Mining (ICDM'2007). 28 – 31 October 2007, Omaha NE, USA. pp. 679-684, IEEE Computer Society, 2007.

- [96] Florian Verhein, Sanjay Chawla: *Geometrically Inspired Itemset Mining*
  IEEE International Conference on Data Mining (ICDM'2006). 18 – 22 December 2006, Hong Kong. pp. 655-666, IEEE Computer Society, 2006.

Other Publications

The following publications constitute research performed by the author in spatio-temporal data mining. They contributed to the author's PhD in the Faculty of Engineering and Information Technology at The University of Sydney, Australia. The thesis was titled "Mining Complex Spatio-Temporal Movement Patterns".

- [92] Florian Verhein. *Mining Complex Spatio-Temporal Sequence Patterns.*
  2009 SIAM International Conference on Data Mining (SDM'2009). April 30 – May 2 2009, Sparks, Nevada, USA. pp. 605-616, SIAM, 2009.

- [99] Florian Verhein, Sanjay Chawla. *Mining Spatio-Temporal Patterns in Object Mobility Databases*
  Data Mining and Knowledge Discovery Journal (DMKD), Volume 16, Number 1 / February, 2008 (online 2007). Springer.

- [90] Florian Verhein: *k-STARs: Sequences of Spatio-Temporal Association Rules*
  IEEE International Conference on Data Mining Workshops (ICDM-W'2006). 18 – 22 December 2006, Hong Kong. pp. 387-394, IEEE Computer Society, 2006.

- [97] Florian Verhein, Sanjay Chawla: *Mining Spatio-temporal Association Rules, Sources, Sinks, Stationary Regions and Thoroughfares in Object Mobility Databases*

The 11th International Conference on Database Systems for Advanced Applications (DASFAA'2006). 12 – 15 April 2006, Singapore. Lecture Notes in Computer Science, Volume 3882, pp. 187-201, Springer, 2006.

- [95] Florian Verhein, Sanjay Chawla. *Mining Spatio-Temporal Association Rules, Sources, Sinks, Stationary Regions and Thoroughfares in Object Mobility Databases*
  IEEE International Conference on Data Mining Workshops (ICDM-W'2005).

Publication Outlet Ranking

At the time of writing, the outlets for the publications listed above were ranked as follows:

Acronym	Conference or Journal Name	CORE'07	ERA'10	MSAS
DATAMINE	Data Mining and Knowledge Discovery journal		A	3
SIGKDD	ACM SIGKDD International Conference on Knowledge Discovery and Data Mining	A+	A	1
ICDM	The IEEE International Conference on Data Mining	A+	A	3
DASFAA	The International Conference on Database Systems for Advanced Application	A	A	9
SDM	SIAM (Society for Industrial and Applied Mathematics) International Conference on Data Mining	A	A	5

CORE'07: Computing research and education association of australasia (CORE) "Final 2007 Australian Ranking of ICT Conferences"[1]. ICT Conferences were ranked in tiers $\{A+, A, B, C\}$. Journals were not ranked.

ERA'10: Since late 2008, journals and conferences are ranked under the Excellence in Research for Australia (ERA) initiative[2]. Conferences were ranked in tiers $\{A, B, C\}$ and journals in tiers $\{A^*, B, C, D\}$. "The A tier for conferences is equivalent to the A^* and A tiers for ranked journals."[3].

MAS: Microsoft Academic Search. Data mining conference and journal ranks by number of in domain citations[4]. January 2011.

[1] Previously available from http://www.core.edu.au/rankings/ConferenceRankingMain.html
[2] Available from http://www.arc.gov.au/era/
[3] http://www.arc.gov.au/era/era_journal_list.htm
[4] http://academic.research.microsoft.com/

Chapter Summary

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Part I

Preliminaries

Chapter 1

Introduction

This chapter introduces and motivates the three main research themes: Generalised interaction mining, statistical approaches in data mining, and mining probabilistic or uncertain databases. These high level research problems are closely linked to each other, primarily through introduction and development of the generalised interaction and rule mining problems and the vectorised computational model and abstract frameworks which can solve a wide range of data mining problems. This chapter provides an overview of this thesis, explains how the problems are linked and how they contribute to the thesis as a whole.

Note: Chapter 2 provides a background on knowledge discovery in databases (KDD) and data mining (DM), and highlights some issues relevant to this thesis.

1.1 Research Problems and Thesis Overview

The research problems addressed in this thesis can be grouped into three main research themes. These are organised into three parts: Part II considers interaction mining problems and proposes novel solutions at the abstract level via generalised frameworks and an efficient vectorised computation model, part III considers the integration of rigorous statistical approaches in novel data mining methods, and part IV proposes and solves the problem of mining probabilistic frequent itemsets in uncertain databases. The sections below introduce and motivate these problems, describe the ways in which they are related to each other as well as providing an overview of the thesis. The primary thread that draws the entire thesis together is the generalised notion of interaction mining: All problems in this thesis can be considered as interaction mining problems. Furthermore, the two main abstract computational frameworks and algorithms – Generalised Interaction Mining (GIM) and Generalised Rule Mining (GRM) – can be used to solve these problems. In fact, they also turn out to be the most efficient solutions.

1.1.1 Generalised Interaction Mining

An interaction is a broad term used in this thesis to describe an effect that variables have on each other, or appear to have on each other. Interaction mining is the process of mining structures on these variables that describe interaction patterns. Usually, these structures can be represented as sets or graphs; where each variable interacts, to some degree, with other variables in the structure. Interactions need not be symmetric or two-way. They may also be complex, which generally means being able to represent both positive and negative relationships, and can include negative patterns. Furthermore, the presence of particular interactions can influence another interaction or variable in interesting ways. These latter kinds of interactions can be expressed as rules – a special type of interaction where an interaction in the antecedent affects a variable in the consequent. Note that interaction mining is unrelated to the research field of human-computer interaction.

Interactions are of interest in domains including social network analysis, marketing, the sciences, to statistics and finance. Furthermore, many data mining tasks can be considered interaction mining, such as clustering (similar objects may be seen to be "interacting"), frequent itemset mining (items bought frequently together suggest these are used together), classification (interactions amongst variables are exploited for prediction or predictive rules capture potentially causal interactions), graph mining (relationships between vertices can be considered interactions) etc.

The Generalised Interaction Mining (GIM) and Generalised Rule Mining (GRM) problems introduced in this thesis are to solve a wide range of interaction mining problems at the abstract level, and to do so very efficiently. This means the problems must be solved at a general level, requiring the development of frameworks and a consistent and efficient computational model that can capture diverse interaction mining problems. This is a challenging task since such problems have very different semantics governing the interactions, their structures and their interpretation. For example, frequent itemset mining, graph mining, finding correlation structures between variables, clustering, rule based classification, mining uncertain databases and mining relationships in social networks (to name a few) have very different problem definitions: The pattern definitions and semantics are different; what makes an interaction pattern interesting is different and how the search should progress is different. The data is also very different; for example, real valued records, a set of time series, transaction databases, probabilistic databases, attribute value pairs produced by discretization, instances and adjacency matrices. Finally, solving interaction mining problems usually requires the simultaneous and interdependent development of new pattern semantics and specialist algorithms for mining the respective pattern. One may therefore conclude that it is not easy to develop a model abstract enough to capture this variation in interaction mining problems, while at the same time enabling the development of an equally abstract algorithm that also solves them efficiently – ideally, more efficiently than specialist algorithms. Doing so is very beneficial however; it can separate the semantics of a problem from the algorithm used to mine it. This makes it easier to develop new methods by allowing the data miner to focus only on their problem's semantics and then plug them into a framework. Furthermore, by removing the burden of designing an efficient algorithm, this can make it easier for end users to design custom data mining methods.

Solving interaction mining problems at the abstract level, as well as applications of this to specific problems, is the primary focus of part II in this thesis.

Chapter 3 introduces and solves the GIM problem. GIM[1] uses an efficient and intuitive computational model based purely on vectors and vector valued functions. The semantics of the interactions, their interestingness measures and the type of data considered are all flexible components. Intuitively, each interaction is represented by a vector in a space typically spanned by the samples in the database. The search progresses by performing functions on these vectors. By providing a layer of abstraction between a problems semantics and the algorithm used to mine it, the computational model allows both to vary independently of each other. It also encourages

[1] Note that the term "GIM" refers both to the problem, as well as the model, framework and algorithm proposed to solve interaction mining problems at the abstract level.

an interesting geometric way of thinking about pattern mining problems in terms of vector operations – especially when an interestingness measure has a geometric interpretation. The GIM algorithm runs in linear time in the number of interesting interactions and uses little space. Chapter 3 also shows how GIM can be applied to a wide range of problems, including graph mining, counting based methods, itemset mining, clique mining, clustering, complex pattern mining, negative pattern mining, solving an optimisation problem, etc.

Chapter 4 presents a vectorised framework and novel algorithm called GLIMIT for solving itemset mining problems from a geometric perspective in a transposed transaction database. It is shown to outperform FP-Growth and Apriori on the frequent itemset mining task. An efficient method for generating association rules is also presented.

Chapter 5 considers the problem of mining complex co-location patterns between different types of objects in a real world spatial database. When applied to a large astronomy database, this mines relationships – including negative relationships and the effect of multiple occurrences – between different *types* of galaxies. Part of this problem can be solved efficiently with GIM or GLIMIT.

Chapter 6 introduces and solves the Generalised Rule Mining (GRM) problem. Rules are an important interaction pattern but existing approaches are limited to conjunctions of binary literals, fixed measures and counting based algorithms. Rules can be much more diverse, useful and interesting! The chapter redefines rule mining in terms of a vectorised computational model similar to that used in GIM. This abstraction is motivated through the introduction of three novel methods addressing problems including correlation based classification, finding interactions for improving regression models and finding probabilistic association rules in uncertain databases. Two of these methods are introduced in chapter 6 (Probabilistic Association Rule Mining (PARM) in uncertain databases and Conjunctive Correlation Rules (CCRules) for classification), while one is introduced in chapter 7.

Since interactions between variables in a database are often unknown to the detriment of further analysis, classification or mining tasks, chapter 7 proposes Correlated Multiplication Rules (CMRules). These capture interactions predictive of a dependent variable and are the first rules with multiplicative semantics. Furthermore, a feature selection and dimensionality reduction method is described whereby CMRules are used to generate composite features. One advantage of this is that it enables linear models to learn non-linear decision boundaries with respect to the original features.

As described in detail below, part II has a strong link to the problems considered in

parts III and IV of this thesis. The methods in part III can be solved[2] efficiently with GIM and GRM: Chapter 8 with GRM and chapter 9 with GIM. Furthermore, GIM turns out to be the most efficient known solution to the probabilistic frequent itemset mining problem considered in part IV. This thesis as a whole therefore validates GIM and GRM's broad applicability, their ability to inspire novel approaches through the vectorised model, the efficiency of their algorithms – even when compared to state of the art approaches for specific problems, and the usefulness of solving problems at the abstract level.

1.1.2 Statistical Approaches in Interaction Mining

Data mining is a hypothesis generating endeavor. DM examines a large database for patterns or interactions that suggest novel and useful knowledge to the user, as defined by a pre-specified interestingness measure. The database itself is a sample drawn or generated from a process, therefore the patterns found should describe hypotheses about the underlying process that generated the data. Furthermore, in searching for these patterns, an algorithm usually makes additional hypothesis pruning the search space as a result of evaluating patterns that the interestingness measure did not rate high enough. Natural questions to ask then, are:

- Does the algorithm find patterns that are significant? That is, are the patterns unlikely to have occurred by chance or sampling effects? Patterns that have a high probability of occurring by chance are misleading since they would not be considered interesting in different samples of the process under consideration. Therefore, decisions based on them cannot be expected to add value to an application relying on that process.
- Did the algorithm make a significant decision during its search? That is, is a decision to prune away part of the search justified or could it have occurred by chance alone?

These questions are often ignored in data mining. It is desirable to provide some minimal level of confidence that the patterns are in fact significant, and do not occur by chance. Even if the data set is not uncertain, it is still a sample generated by a process about which the user wishes to discover knowledge. The knowledge discovered should apply to the process, not the sample database. Nor should it be affected adversely by noise in the database. Furthermore, post processing is not an effective solution to this problem for two reasons: First, it does not address the second

[2] retrospectively

question above. Secondly it means that what the user is ultimately interested in (the knowledge provided at the output of post-processing) is not what the data mining algorithm is searching for. At best, this is very inefficient. At worst, the algorithm never finds those patterns that the post-processing task would rate most highly. In addition to the issue of significant decisions and results, statistics has a range of useful tools and measures that are applicable in data mining. Again, these should be embedded directly into the algorithm rather than applied in post-processing.

Hence, part of this thesis incorporates statistical techniques into novel data mining approaches. The majority of this work is located in part III of this thesis, but some methods are covered in parts II or IV for presentation purposes.

One method employed in this thesis to mine significant patterns is to use significance tests within the interestingness measure. This approach is used in chapter 8, where statistics oriented techniques are combined with a new measure – the Class Correlation Ratio (CCR), for associative classification of standard, and imbalanced data sets[3]. Rules are interesting if they have a positive CCR, are statistically significant and positively associated. The search also progresses based on a significance test and mines significant rules directly. Mining data sets with an imbalanced class distribution is more challenging than in standard data sets, but is required in applications such as medical diagnosis and fraud detection.

A second method to deliver only significant results is to mine patterns that are interesting with a high probability; that is, to generate a significance test around an existing interestingness measure. This approach is taken in chapter 11, where itemsets are mined if they are significantly frequent. This is explained further in the next section.

Due to the inability to make normality (or other) assumptions in many contexts, the focus in this thesis is on non-parametric methods. For example, chapter 8 uses Fisher's exact test, and in chapter 11 calculates the exact probability distribution of support.

Pearson's product moment correlation coefficient is a common statistical tool and is used in a number of novel methods in this thesis. Chapter 9 considers the problem of mining complex maximal cliques of correlated variables (attributes) for the purpose of feature selection, meaningful dimensionality reduction, and as a data mining

[3]Imbalanced data sets have a skewed class distributions. This generally means that there is a large difference in the frequency with which different classes occur. For example, in a database of medical tests, a disease may be present in 5% of cases. In fraud detection, only very few transactions are fraudulent. Despite these low occurrences, it is clearly very important to predict these minority classes. Standard DM and ML approaches generally do not perform well in imbalanced data sets and developing learning algorithms that do is non-trivial.

technique in its own right. Complex interactions consider both positive and negative relationships.

Parts II and III of the thesis are linked in two ways. First, GIM and GRM can be applied to solve parts of the problems in part III; GIM can be applied to mine complex correlation structures and GRM can be used to mine rules based on significance. Secondly, when correlation is incorporated into the vectorised frameworks of GIM and GRM, it has a geometric interpretation as the angle between interaction vectors. This leads to an intuitive method for predictive rule mining where the search causes the antecedent interaction vector to move closer to the vector for the variable to be predicted. This is used in the methods of chapters 6 and 7. Part III is linked to part IV through the development of significant frequent itemset mining in chapter 11.

1.1.3 Probabilistic Frequent Itemset Mining in Uncertain Databases

Association analysis is one of the most important fields in data mining. It is traditionally applied to market-basket databases for analysis of consumer purchasing behaviour, but is much more widely applicable. Such databases consist of a set of 'transactions', each containing the 'items' a customer 'purchased'. The database can be analyzed to discover frequent patterns and associations among different sets of items. The most important step in the mining process is the extraction of frequent itemsets – sets of items that occur in at least $minSup$ transactions. It is generally assumed that the items occurring in a transaction are known for certain, but this is not always the case. In many applications the data is inherently noisy, such as data collected by sensors or in satellite images. In privacy protection applications, artificial noise can be added deliberately in order to prevent reverse engineering of the data through pattern analysis. Data sets may also be aggregated: For example, by aggregating transactions by customer, it is possible to mine patterns across customers instead of transactions. The resulting probabilistic database shows the estimated purchase probabilities per item per customer rather than certain items per transaction.

In such applications, the information captured in transactions is *uncertain* since the existence of an item is associated with a probability. Given an uncertain or probabilistic transaction database, it is not obvious how to identify whether an itemset is frequent because we usually cannot say for certain whether an itemset actually appears in a transaction. This makes the problem challenging.

Prior to the work in this thesis, the expected support was used to solve this problem; an itemset was considered interesting if the expectation of it's support was above

minSup. This approach returns an estimate of whether an object is frequent or not with no indication of how good this estimate is. Since it ignores the probability distribution of support, it can lead to itemsets being labeled frequent even if the probability that they are frequent is less than the probability that they are not frequent. Clearly, this is a problem.

This thesis tackles the problem from a new direction: itemsets are considered interesting if the *probability* that they are frequent is above a user specified threshold τ. This is known as the *frequentness probability*. Accordingly, a *Probabilistic Frequent Itemset* (PFI) is defined as an itemset with a frequentness probability of at least τ.

This creates two main problems:

1. Given the existential probabilities of an itemset in all transactions, how can one efficiently calculate the probability distribution of the support and hence the frequentness probability of the given itemset?

2. How can one mine all itemsets that satisfy the frequentness probability constraints efficiently? This is called the Probabilistic Frequent Itemset Mining (PFIM) problem. A PFIM algorithm has three main tasks: Efficiently searching through the space of uncertain itemsets; efficiently calculating the required probabilities for 1 for each itemset that must be examined; and then using 1 to determine whether an itemset is interesting.

These problems are considered in part IV of this thesis:

Chapter 10 introduces and motivates the PFIM problem as an important research direction. It also solves both parts of the problem: Efficient calculation of the frequentness probability is achieved by employing the Poisson binomial recurrence relation and using a divide and conquer scheme in a possible worlds model. Mining the PFIs is achieved by developing ProApriori; an algorithm based on the Apriori method with candidate generation and testing. An incremental algorithm solving the top k PFI problem is also presented.

Chapter 12 improves on this by developing a probabilistic pattern growth approach inspired by the FP-Growth [47] method. Here, a compact data structure called the probabilistic frequent pattern tree (*ProFP-tree*) compresses probabilistic databases and allows the efficient extraction of the existence probabilities required for part 1 of the problem. The *ProFP-Growth* algorithm is subsequently proposed for mining all PFIs without candidate generation and solves the PFIM problem an order of magnitude faster than ProApriori. Part 1 of the problem is solved in a more intuitive manner by employing generating functions.

Chapter 11 considers the problem of significant frequent itemset mining (SiFIM). Recall from section 1.1.2 that one method of incorporating a statistical test into a data mining algorithm is to test whether the level of interestingness (here, support), is high enough that it is unlikely to have occurred by chance. Both a parametric and an exact method are developed. Additionally, the independence assumption used in PFIM is validated experimentally. Recall that this chapter also provides a link between part IV and III of this thesis.

Chapter 13 shows that the PFIM and SiFIM problems can be solved most intuitively and (by far) most efficiently by employing the GIM framework and algorithm of chapter 3, resulting in the GIM-PFIM algorithm. In particular, the problem naturally maps to the GIM framework by associating a probability vector with each itemset that exists in the subspace spanned by the transactions in which the itemset could exist. This provides an intuitive vectorised view of PFIM. When applied to PFIM, the GIM algorithm solves it orders of magnitude faster, and with an order of magnitude less space than the specialised techniques ProApriori and ProFP-Growth. The evaluation takes place on large, commonly used artificial and real databases. This not only provides the best known solution to PFIM, but further validates the usefulness of the GIM idea and provides a solid link between parts IV and II of this thesis.

1.1.4 Summary of Data Mining Problems Addressed in this Thesis

Within the themes of the above research directions, various data mining problems are considered in this thesis to varying extents. Figure 1.1 provides an overview.

1.2 Publications Contributing to Chapters of this Thesis

This section provides a brief mapping between the chapters in this thesis and the author's relevant publications. Where work is collaborative, it is acknowledged below.

Part I

Chapter 2 contains background material on KDD and DM that is in part derived from the author's PhD thesis at the University of Sydney.

Part II

Problem	Chapter										
	3	4	5	6	7	8	9	10	11	12	13
Generalised frameworks and abstract algorithms for interaction mining	X			X							
Graph mining	X		X				X				
Itemset mining	X	X						X	X	X	X
Association rule mining		X		X							
Rule mining				X	X	X					
Feature selection or generation					X		X				
Classification				X		X					
Mining probabilistic or uncertain databases	X			X				X	X	X	X
Data mining based on statistics (significance tests or correlation)				X	X	X	X		X		
Learning in imbalanced (or skewed) databases						X					
Geometric interpretation of interaction or pattern mining	X	X		X							
Mining spatial databases			X								
Mining negative or complex patterns[4]	X		X				X				
Clustering	X										

Figure 1.1: A summary of problems addressed in this thesis.

Chapter 3 is new and unpublished.

Chapter 4 is based on [96]. It also includes additional material and extended related work.

Chapter 5 is based on [94]. The paper was collaborative work with Ghazi Al-Naymat. A section describing how GIM can be used to solve this problem has also been added.

Chapter 6 is based on [93]. The chapter contains significantly more contributions, examples and details than the publication. For example, the correlation improvement method (e.g. CCRules) does not appear in the paper at all and probabilistic association rule mining (PARM) is only briefly mentioned in the paper. The complexity results are also only briefly men-

tioned in the paper. Furthermore, the framework has been generalised slightly by allowing multiple measures (adding the $k > 1$ and $l > 1$ in section 6.4).

Chapter 7 is new and unpublished. It is closely linked to chapter 6.

Part III

Chapter 8 is based on an extended version of [98]. An analysis of how GRM can be used to solve part of this problem has also been added.

Chapter 9 is based on an extended version of [91]. A section describing how GIM can be used to solve this problem has also been added.

Part IV

Chapter 10 is based on [18] and has been corrected, expanded, reorganised and a uniform terminology introduced. The paper was collaborative work with Thomas Bernecker, Dr. Matthias Renz and Andreas Züfle in Prof. Hans-Peter Kriegel's research group.

Chapter 11 is new and unpublished. It is based on collaborative work with Thomas Bernecker, Dr. Matthias Renz and Andreas Züfle in Prof. Hans-Peter Kriegel's research group.

Chapter 12 is based on [19], which was collaborative work with Thomas Bernecker, Dr. Matthias Renz and Andreas Züfle in Prof. Hans-Peter Kriegel's research group. Additional material has been added and a number of corrections made. For example, the overall ProFP-growth algorithm is included and described. The generating function method for computing frequentness probability was corrected, expanded and new computation and pruning results added.

Chapter 13 is new and unpublished.

Chapter 2

Background

Data is generated from a large number of diverse sources. This data is increasingly being captured with the hope of generating value from the knowledge hidden within it, be this for commercial, scientific, predictive or descriptive purposes. The challenge is how to extract valid, novel, useful and valuable knowledge from the data, do this efficiently and – as much as possible – automatically. Every type of data, as well as the type of knowledge sought from that data, presents its own specific challenges and requirements. This chapter provides a brief background in Knowledge Discovery in Databases (KDD) and Data Mining (DM) and highlights some issues relevant to this thesis.

2.1 Knowledge Discovery in Databases

Data is increasingly being captured because it can – and is – used to better understand the wants and needs of customers; to discover new ways of improving existing practices, products and services; to discover and evaluate new opportunities; to help make better decisions on anything from recommending products to medical diagnosis; to detect and prevent fraud or threats; to automate or make business or other processes more efficient and to help generate, develop and test theories about phenomena. Furthermore, it is becoming established that collected data has value not only for current applications, but also for future but as yet unknown purposes. That is, data is collected for the purpose of obtaining value from the knowledge hidden within it, including for as yet not envisioned applications. The challenge is how to extract this knowledge.

Knowledge Discovery in Databases (KDD) attempts to solve the problem of extracting knowledge from data (typically stored in databases) and to provide valuable information to the user. It aims to do this – as much as possible – automatically. This information should be "valid, novel, potentially useful, and ultimately understandable" [36]: It should capture valid information and be applicable to new data, rather than capturing an artifact that occurred by chance. It should be non-obvious and represent new information for the user. It should also be understandable and ultimately usable to improve a given application, system or process. Extracting this sort of information from large quantities of data is a valuable but often difficult proposition.

While KDD concerns itself with information discovery, not all information discovery tasks constitute KDD. For example, retrieving individual customer records or querying a database management system or search engine are primarily Information Retrieval (IR) problems. IR is the science of searching for information to answer specific queries. Since the information being sought is well defined and typically understood, the problem is to efficiently search for those documents or records that contain the desired information. KDD on the other hand, aims to find knowledge that the user did not know existed or does not yet understand. Furthermore, this knowledge is typically more structured, complex and abstract. For example, rather than finding web pages on a particular topic, KDD and data mining applied to the world wide web (known as "web mining") may find information such as a hierarchical description or taxonomy of topics and their relationships to each other, the structure of web pages or patterns in the way web pages are used and how this changes over time. On the other hand, similarity search is a key component in both information retrieval and clustering, the latter being a data mining method that finds groupings

of objects that are similar to each other. KDD is a multi-disciplinary field and often overlaps IR, Machine Learning (ML), statistics, algorithms, databases, probability theory and theoretical computer science. Some aspects which differentiate it from other fields are its attention to exploratory analysis, the ability to find and evaluate complex patterns, its usefulness for hypothesis generation and its applicability to massive data sets.

Knowledge Discovery in Databases has many challenges including:

- Data sets are typically large which makes efficiency and scalability important in order to deliver results to the user in an acceptable time frame. In particular, the data sets considered in KDD are typically much larger than those considered in ML. This often makes non-trivial problems that overlap the database field important, such as the storage, efficient access to and indexing of data.
- Data sets often have a high dimensionality. Methods developed for low dimensional data are usually not applicable to high dimensional data since data becomes sparse, distances between data points become similar and the effect of noise is amplified. Furthermore, the computational cost of many analysis methods increases rapidly with the number of dimensions.
- Data is becoming increasingly complex and heterogeneous. For example, data instances may be graphs or multi-instance objects and attributes may be a mix of continuous, discrete, and semi-structured data.
- It is typically not known what information is sought prior to the application of KDD. Hence KDD is hypothesis generating and exploratory in nature, in comparison to traditional statistics for instance where an important task is testing hypotheses constructed by a knowledgeable user.
- The type of knowledge sought by KDD is non-trivial and often involves complex structures, descriptions and relationships. This leads to large search spaces which demands efficient solutions, as will be discussed in section 2.2. OLAP, in contrast, is suited to computing and visualising the entire data set or relatively simple aggregates, projections and groupings of records to find things such as customer purchasing trends. Similarly, hypotheses in statistics are typically simpler.
- Since KDD is a practical endeavor, it must consider real world issues such as noise, uncertainty and faults within the data. Ignoring these can adversely impact the ability to extract valid knowledge or lead to misleading results.

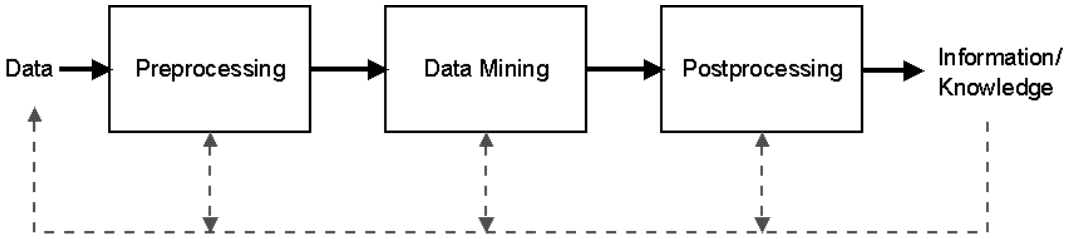


Figure 2.1: The classic view of the Knowledge Discovery in Databases (KDD) process. Solid arrows represent the flow of Data through the KDD process, while the dotted arrows show the typically iterative process through which a KDD application is designed.

The classic framework for KDD attempts to separate some of these challenges. As illustrated in figure 2.1, the KDD process consists of three steps: data pre-processing, data mining and post-processing of the results.

1. Data **pre-processing** collects, selects and transforms the raw data into an appropriate format for subsequent analysis. It includes tasks such as: Data aggregation from multiple and potentially distributed sources; data selection or sub-setting to obtain the relevant features (typically columns) and samples (typically rows); normalization of the data to avoid feature biases (for example, differing scales impact distance based data mining algorithms); data "cleaning" in an attempt to remove noise, duplicate records or outliers; application specific methods for dealing with missing data (for example, should missing data be ignored or treated as meaningful?); data transformation into a suitable format; feature extraction; feature processing (for example, discretization); and dimensionality reduction methods (for example, Principal Component Analysis).

2. **Data mining** is the task of efficiently finding potential knowledge, or *patterns*, in the preprocessed data (Data Mining will be properly defined and discussed in section 2.2). This is the most important and challenging step in the KDD process. It includes the selection or development of a DM algorithm that is appropriate for the type of knowledge desired and is able to find interesting patterns in an acceptable time frame. Furthermore, setting relevant parameters for the algorithms is a non-trivial task.

3. **Post-processing** attempts to ensure that only valid, useful and understandable results are delivered. It includes tasks such as filtering, ranking, visualization of results, validation and verification to remove spurious results – perhaps using statistical methods – and interpreting the patterns found by DM.

While DM itself is automated, many of the pre- and post-processing tasks require some human input and domain knowledge in order for the KDD process to be successful. For example, domain knowledge is often required for effective feature selection. Similarly, the output of data mining algorithms cannot simply be assumed to be valid. The additional steps in the KDD process are essential to ensure that useful and valid knowledge is derived from the data. Blind application of data-mining methods is a dangerous activity and easily leads to the discovery of meaningless or outright invalid patterns [35]. The reason for this is that one can find, for example, statistically significant patterns in any data set – even a randomly generated one – if one searches long enough. Other problems such as noise, incorrect or lack of normalization, careless selection of features or failing to consider outliers can also lead to invalid patterns being found. These difficulties typically lead to an iterative KDD process, illustrated in figure 2.1 by the dotted arrows, where the results of all three steps in the KDD process feed back into the decisions made in the previous stages.

The interested reader is directed to [35] for a more in depth introduction to the high level KDD process. While as of this writing the article is over 13 years old and the field has progressed considerably, it provides a good overview and definitions of KDD, the classic KDD process, its relationship to longer established fields like artificial intelligence, machine learning, statistics and databases, as well as some early real world applications. For more concrete information about the various tasks and algorithms in the KDD process, the reader is directed to [88] and [46] which provide excellent introductions.

2.2 Data Mining

Data Mining (DM) is the most important and complex component of the KDD process. There are a number of "definitions" of data mining. The following is most closely related to that of [88], with the primary difference being the use of the term pattern instead of information[1].

[1] This is for two reasons: First, the author prefers the more concrete term "pattern" since, as shall hopefully become clear in the text, this leads to a natural way of explaining and understanding the data mining process. Secondly, the author doesn't think that patterns (or to be more specific, pattern instances in the terminology introduced here) necessarily qualify as information or knowledge. Patterns are the output of an automated process which together, perhaps after post processing, visualization, validation or human interaction, may become information. It should be noted that "pattern" is usually used in the literature in the context of association rules and itemset mining, for example "frequent pattern mining", but that patterns are not restricted to this sub-field. Pattern is also used in the definition of data mining by [35].

Definition 2.1. Data mining is the automated process of extracting useful patterns from typically large quantities of data.

Different *types* of patterns capture different types of structures in the data: A pattern may be in the form of a rule, cluster, set, sequence, graph, tree, etc. and each of these pattern types is able to express different structures and relationships present in the data. For example, a rule may tell a marketer about strong relationships between purchased goods or services, predict customer 'churn' or be used as the basis of recommender systems. A set can indicate products that customers are purchasing together and a cluster might tell him or her about groups of customers that have similar purchasing patterns. These may be used as the basis for a marketing scheme that aims to maximize response rates and sales for a given investment. A graph may tell a biologist about strong and previously unknown gene or protein interactions present in their experiments, or a security agent about suspicious communication structures between potential criminals. A tree or a set of rules may describe the decision structure that can be used to accurately predict medical conditions, perhaps based on patient records or medical imaging data. As suggested by these examples, patterns can be *descriptive* or *predictive* (or both). That is, they can be used to describe, model and help better understand a process or phenomena or to predict future events. In this work, many new types of patterns are introduced. Some are purely descriptive and some are explicitly used for prediction purposes.

Once a pattern type has been defined based on the problem at hand and the structure of the information sought, the goal – and challenge – is to automatically find those pattern *instances*[2] in the data that are interesting to the end user. That is, pattern instances providing both useful and previously unknown (novel) information. This is done by evaluating pattern instances for interestingness according to some measure that, ideally, should model the value that the user obtains from being made aware of the pattern. An *interestingness measure* measures how interesting a pattern instance is expected to be. These measures must balance three important characteristics:

1. The **utility** that a user is expected to receive by exploiting the pattern instance. For example; the value, financial gain, increase in accuracy or efficiency or

[2]In the terminology used here, a pattern type describes the structure or schema of the pattern. For example, an itemset can be defined as a non-empty subset of all items that may be purchased in a supermarket. This specifies its type. A pattern instance on the other hand is a particular instantiation of that type. For example, $\{bread, butter, jam\}$. A pattern therefore has one type but many instances, and these instances are "found" in the data set. This distinction between type and instance is rarely made explicit but helps to describe the data mining process in terms of the definition used in this thesis. In the literature and common usage, the term "pattern" is inherently ambiguous and refers to both or either the type or instance, depending on the context. Outside this section, the term will typically refer to the pattern instance of the type being discussed.

ability to understand a phenomena. Modeling utility directly is usually too difficult in practice and simpler but objective measures are used instead, ideally with reasoning linking them back to the users expected utility.
An important influence on the utility of pattern instances is how many of them are labeled as interesting. The utility that a user gains from the results of data mining – namely, the set of all pattern instances mined – can easily fall if too many results are delivered, especially if many of them are similar. One way of combating this problem is post-processing the results. Another method, favoured in this thesis, is to mine interesting patterns directly, mine only statistically significant patterns or patterns with a high probability of being interesting.
Finally, utility should also attempt to capture *valid* patterns, as opposed to spurious ones. This is a motivation for the probabilistic and statistical methods employed in parts of this thesis.

2. The **novelty** of the pattern instance. For example, simple patterns may be useful or describe a strong relationship but if they are already known or obvious then they provide no added value. Novelty is difficult to take into account, but a simple method to counter obviousness is perhaps to ensure that a user is directed to larger or more complex patterns in favour of simple ones.

3. The **complexity** of calculating the measure and searching for those pattern instances that have a high interestingness value. Usually, the goal is to develop a *complete* algorithm (if possible) so that all patterns satisfying a particular interestingness criteria will be found. Sometimes this is possible even in very large databases as some measures allow a suitably developed algorithm to prune away most of the search space. However, in other cases it is intractable to find all interesting results. In such cases, it is possible that approximate, heuristic or probabilistic methods can be employed. These limit the search space and complexity while still delivering useful results. The downside is that the user is never completely sure that all pattern instances that may be of interest to him or her are found, or that the best or optimal pattern is found. On the other hand, this is usually better than not being able to deliver any results. The complexity of the resulting algorithm and properties that may be exploited are therefore an important consideration in designing an interestingness measure.
One of the results of this thesis is that forcing good quality interestingness measures (that correlate with the users utility) to be anti-monotonic (this enables efficient pruning) when they do not naturally have pruning friendly properties gives much better results than using interestingness measures that allow

pruning but are not directly related to the users utility.

With a type of pattern and interestingness measure defined, the challenge is to develop an efficient algorithm to find the interesting pattern instances in large data sets. Of course, as hinted above, this may be an iterative process where the design of the algorithm and interestingness measures affect each other.

One of the contributions in this thesis is the development of generalised algorithms, frameworks and a computational model that separates the semantics of the patterns and interestingness measures from the algorithm used to mine them. This makes the design process much easier, as both problems can be solved independently. Furthermore, the ability to plug in interestingness measures into an efficient framework and algorithm allows the data miner to focus on the semantics of the problem.

Part II

Generalised Interaction Mining

Chapter 3

Generalised Interaction Mining

Interaction mining is the process of mining structures on variables that describe how they interact (or appear to interact) with each other. Generalised Interaction Mining (GIM) is a model, framework and algorithm that solves interaction mining problems at the abstract level. The semantics of the interactions, their interestingness measures and the type of data considered are flexible components. An efficient and intuitive computational model based on vectors and vector valued functions is developed. This functions as a layer of abstraction between a problems semantics and the algorithm used to mine it; allowing both to vary independently. It encourages a geometric way of thinking about pattern mining problems in terms of vector operations and subspaces. It allows new methods to be developed by focusing purely on the problem's semantics. The GIM algorithm requires minimal space and runs in linear time in the number of interesting interactions found.
The GIM framework and algorithm are a cumulative result of many problems that the author has solved. In addition to introducing GIM, this chapter demonstrates the breadth of problems that are solvable with GIM by showing how it can be applied in diverse applications.

3.1 Introduction

An interaction is a broad term used in this thesis to describe an effect that variables have on each other, or appear to have on each other. Interaction mining is the process of mining structures on these variables that describe interaction patterns. Usually, these structures are represented sets or graphs; where each variable interacts, to some degree, with other variables in the structure.

Many domains can benefit from the application of interaction mining. In social networks people interact with each other through personal contact, email, instant messaging, telephone and social network applications. Social network analysis is used in applications such as understanding how patterns of human contact affects the spread of diseases, surveillance and counter intelligence operations, understanding the spread of ideas and for marketing and promotion. In marketing, different promotional campaigns and customer facing services interact to affect customer retention and the bottom line. In pharmacology, drugs may interact with each other. In genetics, genes interact with each other to affect the phenotype (observable characteristics) of organisms. In statistics, interactions between variables create effects greater than the individual variables would, or may be measured by correlation or significance tests. In finance, equities interact (or appear to interact) with each other as reflected by similarities in the time series of their prices. In ecology, movement of animals over time may show behavioural interactions. Such interactions may be complex and include both positive and negative interactions. For example, signed graphs in social network analysis can show friendship or aversion; there are additive or suppressive actions between drugs or genes; and mining positive an negative correlations between variables could reveal useful patterns in a range of applications. Furthermore, many data mining tasks can be considered as mining interactions, such as clustering (similar objects may be seen to be "interacting"), frequent itemset mining (items bought frequently together suggest these are used together), classification (interactions amongst variables are exploited for prediction), spatio-temporal data mining techniques (flocks and other co-location patterns describe interactions between objects), etc. Mining interactions between variables is therefore a general data mining concept that covers a range of problems.

However, these problems have very different semantics governing the interactions, their structures and their interpretation. Naturally, these problems all have different definitions of what it means for an interaction pattern to be interesting or useful. The

problems also have very different types of data, such a real valued records, a set of time series, transaction databases, attribute value pairs produced by discretization, instances and adjacency matrices. Usually, solving such problems requires the simultaneous and interdependent development of new pattern semantics and specialist algorithms for mining the respective pattern.

Generalised Interaction Mining (GIM) is a framework and method for mining interactions at the abstract level. It does this by leaving the semantics of the interactions, the interestingness measures used to evaluate the interactions and the data types in which the interactions are to be mined as flexible components. This creates a layer of abstraction between a problem's definition/semantics and the algorithm used to solve it. Instantiations of GIM solving specific problems need only specify these abstract components, and the GIM algorithm can be used to mine all interesting interactions satisfying these constraints. This is achieved by developing a consistent but general computation model based on vectors and vector valued functions, where each interaction is represented by an *interaction vector* in some space X. This framework is able to capture a wide range of interaction mining problems simply by instantiating these functions in different ways. Since the framework operates as an interface between the semantics of a problem and the algorithm used to mine it, this abstraction layer enables the problem's semantics and algorithm to vary independently of each other. This means that new methods can be developed by focusing on the semantics of the problem, without being concerned with how these semantics are mapped to a new algorithm. As long as the semantics of the problem can be mapped to the framework – and it will be shown in this chapter and thesis that many can – the GIM algorithm can solve it efficiently. Similarly, since the algorithm depends only on a set of abstract vector valued functions, it is independent of the semantics of the particular instantiation and can be swapped out – for example should a more efficient one become available, to cater for different trade-offs between time and space resources or to leverage different computation architectures.

GIM's computational model also provides an intuitive "geometric" way of thinking about problems, as it requires them to be cast into vectors and vector valued functions. Every interaction is represented by a vector, called an *interaction vector*, in a high dimensional space X typically spanned by the samples recorded in the database. By combining such vectors, larger interactions can be built, with vectors typically existing in subspaces of X. By evaluating functions over these vectors, the interestingness of interactions can be computed.

The GIM algorithm operates purely by using these functions on interaction vectors, and searches the space of possible interactions in the most space and time efficient

method possible. This means that interaction vectors are never created more than once but are reused, while at the same time ensuring that the minimum number of interaction vectors are in memory at one time. The space required is provably linear in the size of the data set. The run-time is provably linear in the number of interactions that need to be examined. These properties allow it to outperform specialist algorithms when applied to specific interaction mining problems, such as frequent itemset mining and probabilistic frequent itemset mining. Furthermore, the vectorization inherent in the framework's functions provides additional avenues for reducing the run time: On single processor architectures, vectorization allows automatic parallelisation and exploitation of machine level operations for bit-vectors. On multiprocessor architectures, vectorization also provides a point for concurrentisation [105] while on supercomputer architectures, single instruction vector processing is directly supported [105].

3.1.1 Relationship to other Chapters

The approach described in this chapter was developed over an extended period of time while solving other research problems efficiently and discovering similarities in the way these problems could be solved. While other chapters in this thesis present problems that can be solved (retrospectively) using the GIM framework, this may not have been done at the time. This is also one of the last chapters that was written and therefore also functions as a broad treatment of interaction mining and generalised pattern mining. Accordingly, the emphasis is on the abstract framework, the GIM algorithm and presenting a sample of the many problems to which it can be applied. Other chapters evaluate some of these problems in depth and therefore demonstrate the superiority of applying GIM to specific research problems. This is described in section 3.16.

Chapter 6 extends the concept of interaction mining to rules, introducing and defineing the generalised rule mining (GRM) problem. This allows the capture of patterns where an interaction in the antecedent affects a variable in the consequent. This can be used to find patterns where interactions have seemingly causal effects on other variables, in particular enabling predictive patterns to be found. For example, in marketing, various promotions, incentive programs and media coverage interact to affect consumer behaviour, such as the number of new customers, customer churn or customer spend. Like GIM, GRM solves problems at the abstract level.

3.1.2 Contributions

This chapter makes the following contributions:

- It introduces the Generalised Interaction Mining (GIM) problem and presents an abstract framework that allows interaction mining problems to be specified in terms of functions on interaction vectors. This framework separates the semantics of interaction mining problems from the algorithms used to mine them, provides a generic computational model for solving GIM problems and a useful geometric way of considering these problems in terms of vectors and subspaces.
- It presents the GIM algorithm, which is able to solve any problems expressed in the GIM framework efficiently. It is proved to have linear run time in the interesting interactions found and uses space linear in the size of the database (usually less). Extensions are also developed for solving a range of complex problems.
- It shows that GIM can be applied to solve a wide variety of existing and novel problems.
- Section 3.12.1 proves that the $maxPI$ measure, used in spatial data mining, is anti-monotonic under an ordering of variables. Previously this was thought to be weakly anti-monotonic. This leads to an more efficient solution using GIM.

3.1.3 Organisation

The remainder of this chapter is organised as follows. Section 3.2 presents the Generalised Interaction Mining (GIM) framework. Section 3.3 presents the GIM algorithm. Subsequent sections show how diverse problems can be mapped to the framework and solved by GIM; and how, through various extensions, GIM is able to solve more complicated problems.

3.2 Generalised Interaction Mining Framework

This section presents the vectorised GIM framework. Let $V = \{v_1, v_2, ..., v_m\}$ be the set of *variables* about which interaction information is desired. The data is said to consist of a set of *samples* $\{s_1, s_2, ..., s_n\}$ capturing the variable's values. The goal is to find *interesting* subsets of V, where these subsets $V' \subseteq V$ – corresponding to

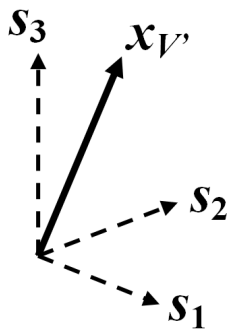


Figure 3.1: An interaction V' visualised as a vector $x_{V'}$ in the space X of (3) samples.

interactions – can have any given semantics and structure. Each possible interaction $V' \subseteq V$ is expressed as a vector, denoted by $x_{V'}$ and called an *interaction vector*. These vectors exist in a space X, the dimensions of which are typically[1] the samples recorded in the data set. This is illustrated in figure 3.1. Depending on the application, samples may be instances, transactions, rows, points, objects located in some space, successive values in time-series, entries in a correlation matrix, etc. In general, each sample captures the value that each of the variables had when that sample was recorded. Conceptually then, the database D consists of the set of interaction vectors corresponding to individual variables, $D = \{x_v : v \in V\}$, where the entry $x_v[i] : i \in \{1, n\}$ records the value of v in the ith sample (dimension). Note that interaction vectors need not be implemented as vectors or arrays as suggested here; they only need to capture the information describing the interaction in the samples; and all interactions – including single variables – must be able to be represented by vectors in the same space X. The space X is dependent on the type of variables considered. For example, in itemset mining the space is the hypercube $\{0, 1\}^n$ since each item is either contained or not contained in any of the n transactions, while in clustering, clique or graph mining the space may be $\mathbb{R}^n$. Variables may be mixed type, or may even be vector or graph valued if required. The semantics of the interactions V' are also variable; they may be conjunctive as in frequent pattern mining, they may represent cliques of other types of sub-graphs in graph mining applications, or may simply be a set of variables that have some type of dependency or correlation with each other. Recall that examples of a wide range of interactions supported by the framework will be presented later in this chapter.

[1] Sometimes it is useful to store additional information in order to make the algorithm more efficient. One example of this is described in section 3.12.1.

The first component of the framework is an order on the variables.

Definition 3.1. The variables $v \in V$ have a *strict total order* $<$ defined on them. Write $v_i < v_j \iff i < j$.

This is trivially satisfied in most applications as variables occur in some arbitrary order in the data set, and the order does not impact on the resulting patterns. In some applications a particular order is important. For example, section 3.12 shows that the $maxPI$ measure is anti-monotonic provided that variables have a particular order.

Since each interaction V' is represented by a vector $x_{V'}$ in X, the evaluation of that interaction is performed with a vector valued function $m_I(\cdot)$.

Definition 3.2. $m_I : X \to \mathbb{R}^k$ is a measure on a vector $x_{V'}$. $m_I(x_{V'})$ evaluates the quality of the interaction V'. k is fixed.

That is, m_I evaluates an interaction based only on the information available in that interaction's vector. $k \geq 1$ allows the function to evaluate V' according to multiple criteria.

.

In order to evaluate an interaction with $m_I(\cdot)$, its interaction vector must first be built. Recall that the data set contains all x_v where $v \in V$ are the single variables. The interaction vectors $x_{V'}$ with $|V'| > 1$ are built incrementally using the *aggregation function* $a_R(\cdot)$, which maps two vectors in X onto X:

Definition 3.3. $a_I : X^2 \to X$ operates on interaction vectors so that $x_{V' \cup v} = a_I(x_{V'}, x_v)$ where $V' \subset V$, $v \in (V - V')$, and v occurs prior to all elements in V'. That is, $v < v' \forall v' \in V'$.

In other words, $a_I(\cdot)$ combines the vector $x_{V'}$ for an *existing* interaction $V' \subset V$ with the vector x_v for a new variable $v \in V - V'$. The resulting vector $x_{V' \cup v}$ represents the larger interaction $V' \cup v$. In this way, vectors representing interactions can be built incrementally. Note that the resulting vector is the same as if it were calculated

from the original data set, but rather than examining the original data set for all $v' \in V' \cup v$, it requires only one of the vectors (x_v) as the information from the rest is already represented in $x_{V'}$. This is exploited by the GIM algorithm, allowing it to efficiently evaluate interactions without recomputing vectors or scanning the data set. Note that $a_I(\cdot)$ need not be commutative, even though the subscript $x_{V' \cup v}$ uses set notation for simplicity. Furthermore, note that the order can be used in applications for semantic purposes, as it is guaranteed that interaction vectors are built in a particular and fixed order.

Note that implicitly, $a_I(\cdot)$ *defines the semantics of the interaction.* By defining how $x_{V' \cup v}$ is built, it must implicitly define the semantics between variables in the interaction. That is, what it *means* to add a variable to the existing interaction V'.

Example 3.4. The simplest interaction mining approaches counts the number of samples that exhibit an interaction V'. In these cases, the interaction vector semantically consists of the set of samples that contain the interaction and $m_I(\cdot)$ is simply the size of this set. $a_I(\cdot)$ is the intersection operation, so that all variables must be present in a sample for it to be counted. This leads to conjunctive semantics.

While $m_I(\cdot)$ and $a_I(\cdot)$ are sufficient in a number of applications, it sometimes occurs that an interaction V' needs to be compared with its *sub-interactions* $V" : V" \subset V'$ in order to compute an interestingness measure. There are a number of problems in this thesis where this is required, including mining spatial co-location patterns. Furthermore, it allows the explicit measurement of how much an interaction V' improves over its more general sub-interactions $V" : V" \subset V'$, a topic that will be considered in depth in section 3.21. The following function supports such behaviour.

Definition 3.5. $M_I : \mathbb{R}^{k \times |\mathcal{P}(V')|} \rightarrow \mathbb{R}^l$ is a measure that evaluates an interaction V' based on the values computed by $m_I(\cdot)$ for V' or any sub-interaction $V'' : V'' \subset V'$. l is fixed.

Like $m_I(\cdot)$, $M_I(\cdot)$ may compute multiple values. $M_I(\cdot)$ does not take vectors as arguments – it evaluates a rule based on values that have already been calculated by $m_I(\cdot)$. This is for algorithmic efficiency purposes and does not limit the scope of the framework. If $M_I(\cdot)$ does not need access to any sub-interactions to perform its evaluation, it is called *trivial* since $m_I(\cdot)$ can perform the function instead. A *trivial* $M_I(\cdot)$ simply returns $m_I(\cdot)$ and leads to reduced run time and space usage by the algorithm, as will be described in section 3.3.

The final component of the framework defines what interactions are *interesting*. Interesting interactions are

1. Desirable and should therefore be output to the user and
2. Should be further expanded in the sense that additional variable should be added in order to grow the interaction.

For flexibility, these two concepts may be separated.

Definition 3.6. $S_I : \mathbb{R}^{l+k} \rightarrow \{true, false\}$ determines whether an interaction V' should be expanded or the search should stop at this interaction. This is determined based on the values previously computed by $m_R(\cdot)$ and $M_R(\cdot)$.

In other words, more specific interactions – That is, larger interactions with more variables – will only be considered if $S_I(\cdot)$ returns true. Independently, the interestingness to the user is defined as follows;

Definition 3.7. $I_I : \mathbb{R}^{l+k} \rightarrow \{true, false\}$ determines whether an interaction V' is *interesting* based on the values computed by $m_R(\cdot)$ and $M_R(\cdot)$. Only interesting rules are output by the algorithm.

Note that an interaction may be interesting according to $I_I(\cdot)$ but not according to $S_I(\cdot)$. This means the interaction will be output, but no larger interaction will ever be examined or output. Conversely, an interaction may not be interesting according to $I_I(\cdot)$ but if $S_I(\cdot)$ returns true, then larger interactions will be examined, some of which may be interesting according to $I_I(\cdot)$. Of course $I_I(\cdot)$ and $S_I(\cdot)$ may be identical. The simplest implementation of either function is to return true if one of the values computed by $M_I(\cdot)$ or $m_I(\cdot)$ is above a threshold.

Note that this framework accommodates approaches where an interaction V' is examined after its sub-interactions $V'' \subset V'$. That is, bottom up approaches. It is possible to accommodate top-down approaches be inverting the problem, as described in section 3.7.

An additional function $P_I(x_{V'}, v)$ (definition 3.17) that allows early pruning and thus avoids computing vectors in some applications will be considered in section 3.8. An additional function $N(\cdot)$ (definition 3.13) can be included for supporting negative patterns and will be discussed in section 3.6. The subscripts I in the functions in this framework is used to differentiate them from related functions in the Generalised Rule Mining (GRM) framework, covered in chapter 6.

3.3 Generalised Interaction Mining Algorithm

This section presents the Generalised Interaction Mining (GIM) algorithm, which solves any problem expressible in the GIM framework efficiently. First, an important data structure is presented.

3.3.1 Prefix Tree

In order to make the algorithm easy to understand, a *prefix tree* will be used to help describe it, prove properties, and in some cases, to store a collection of interactions in compressed form.

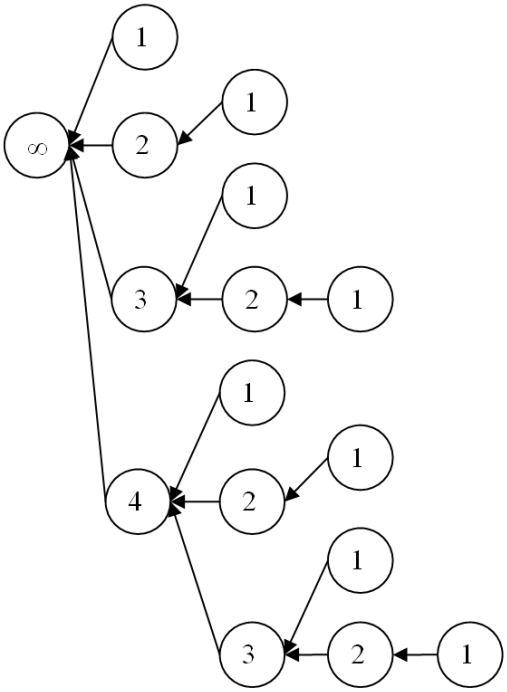
Since all variables $v \in V$ have a strict total order (definition 3.1), they can be mapped to the set of integers. Without loss of generality therefore, assume the variables are integers $V = \{1, 2, ..., |V|\}$. An interaction can therefore be represented as a sequence of integers, ordered in decreasing order according to $<$ (definition 3.1). A space efficient way to store a collection of interactions (in those cases when this is necessary) is to share common prefixes in a tree structure. An example of a prefix tree is shown in figure 3.2(b).

In a prefix tree ($PrefixTree$), each node – called a $PrefixNode$ – has a label corresponding to a variable $v \in V$ (this will be called $variableId$ in algorithm 3.1). The root node is special, and is labeled with ∞. The tree is constructed so that each node can only have a parent with a label greater than it's own label. Each node has a reference to its parent, but not to its children. Maintaining only parent links is used to increase the run time and space efficiency of the algorithm. It also sets it apart from a Trie [66] data structure. In particular, in many instantiations of the framework, only a single branch (path toward the root) of a prefix tree must ever be retained in memory at one time. In a prefix tree, two nodes are called *siblings* if they share the same parent. Each $PrefixNode$ represents a distinct subset of the variables and as such represents a unique interaction. The interaction can be re-constructed efficiently by traversing toward the root. The root node corresponds to the empty interaction. Each node also contains the values computed by $m_I(\cdot)$ (called $value_m$), $M_I(\cdot)$ (called $value_M$) and $I_I(\cdot)$ (called $interestingness$). It is not necessary to store the result of $S_I(\cdot)$.

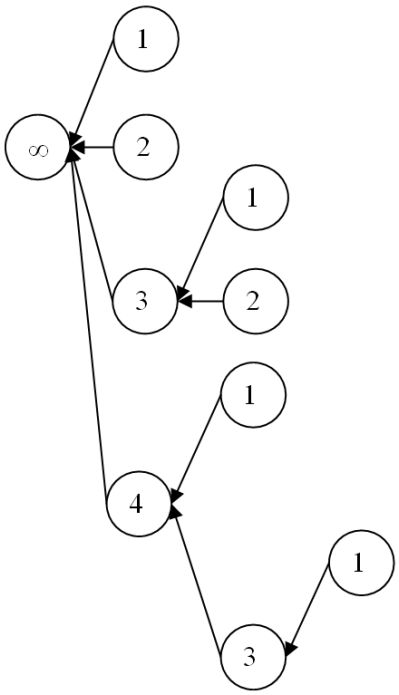
A "complete" prefix tree is a tree containing all possible interactions. Therefore, it also represents the worst case search space of GIM and contains exactly $2^{|V|}$ nodes. An example of a complete $PrefixTree$ is given in figure 3.2(a).

Algorithm 3.1 The basic Generalized Interaction Mining (GIM) algorithm. It employs a strict depth first search with backtracking. For simplicity, a garbage collector is assumes to clean up nodes that are no longer required. Functions not defined here are $outputInteraction(\cdot)$, $store(\cdot)$ and $evaluateM_I(\cdot)$. These latter two are required for non-trivial $M_I(\cdot)$. For trivial $M_I(\cdot)$, $evaluateM_I(newNode)$ simply returns $newNode.value_m$. The simplest implementation of $outputInteraction(newNode)$ simply traverses from $newNode$ toward the root and outputs the sequence of $variableIds$ found along the way. It can be used to implement functionally useful operations too however, as will be shown later.

```
//Data Structure
//The nodes that constitute the PrefixTree.
class PrefixNode{
 PrefixNode parent,
 String variableId,
 double[] value_m,
 double[] value_M,
 boolean interesting};

//Initialisation
PrefixNode root = new PrefixNode(null, ε, NaN, NaN, false);
Vector x_∞ = ... //initialise appropriately (e.g. all ones)
List joinTo =
... //set of all variables, ordered according to <.
GIM(root, x_∞, joinTo);

//node: The PrefixNode corresponding to the interaction V' that
//   should be expanded using the variables in joinTo.
//joinTo: Contains contains individual variables.
//x_V': The interaction vector corresponding to V'.
GIM(PrefixNode node, InteractionVector x_V', List joinTo)
 List newJoinTo = new List();
 PrefixNode newNode = null;
 for each v ∈ joinTo
  Vector x_V'∪v = a_I(x_V', x_v);
  double[] value_m = m_I(x_A'∪v);
  newNode = new PrefixNode(node, v, value_m, NaN, false);
  double[] value_M =evaluateM_I(newNode);
  newNode.value_M = value_M;
  if (I(value_m, value_M))
   newNode.interesting = true;
   outputInteraction(newNode);
  if (S(value_m, value_M)) //expand the search
   if (M_I(·) is non-trivial)
    store(newNode);
   GIM(newNode, x_V'∪v, newJoinTo); //recursive call
   newJoinTo.add(v);
```



(a) A *complete* prefix tree with variables $V = \{1, 2, 3, 4\}$. A complete prefix tree contains all possible combinations of the variables.



(b) An example of a prefix tree with variables $V = \{1, 2, 3, 4\}$ containing the following interactions: $\{\{1\}, \{2\}, \{1, 3\}, \{3\}, \{2, 3\}, \{1, 4\}, \{4\}, \{1, 3, 4\}, \{3, 4\}\}$

Figure 3.2: Prefix tree examples. Note that the prefix tree does not need to be stored in memory unless access to sub-interactions is required by $M_I(\cdot)$. This is covered in section 3.11.

3.3.2 Algorithm

The GIM algorithm (algorithm 3.1) works by performing a *strict* depth first search with backtracking (note the recursive call inside the for loop occurs for every single variable in *joinTo*). This means that sibling nodes are not expanded until absolutely necessary. For example, in figure 3.2(a) the entire sub-tree under the path $\langle 4, 2 \rangle$ (i.e. $\langle 4, 2, 1 \rangle$) is completely expanded before the interaction corresponding to $\langle 4, 3 \rangle$ (and its corresponding $PrefixNode$ and interaction vector) is even built or considered. Child nodes are expanded in increasing order (order is always maintained without sorting) and their corresponding interaction vectors are calculated along the way. There is no candidate-generation, as each new interaction is evaluated by $m_I(\cdot)$ and $M_I(\cdot)$ immediately after it is created and before any other nodes are created or examined. The search is limited according to the interestingness function $S_I(\cdot)$, which stops the search along a branch. The search progresses in depth by *joining sibling nodes*

in the $PrefixTree$, so to speak. This means that an interaction $\langle 4,3,2\rangle$ is created by joining the siblings $\langle 4,3\rangle$ and $\langle 4,2\rangle$. Note however that while $joinTo$ contains individual variables, it only contains those that correspond to the last variable in siblings of the node being expanded. This auto-prunes the search, since $\langle 4,3,2\rangle$ can only be created if the sibling $\langle 4,2\rangle$ exists (is was found to be interesting according to $S_I(\cdot)$). If $\langle 4,2\rangle$ was not found to be interesting, then $\langle 4,3,2\rangle$ would never be considered. This auto pruning is useful for measures that are anti-monotonic or weakly anti-monotonic. Should this be undesirable, it can be easily disabled by placing the last line of the algorithm outside the `if` $(S(value_m, value_M))$ statement.

Vectors are calculated incrementally along a path in the search using $a_I(\cdot)$. This is done in a way so that there are never any vector re-computations while at the same time maintaining optimal memory usage. To appreciate this, consider the alternatives: One option is to calculate each interaction vector from the vectors for single variables when it is needed. While this requires no additional space, it requires $|V'|$ applications of $a_I(\cdot)$ to create $x_{V'}$ and many re-computations of the same vector (vectors for prefixes would need to be recomputed), which is clearly undesirable. Another alternative is to keep many interaction vectors in memory and add variables to these with $a_I(\cdot)$ when needed, so that it is guaranteed that only one application of $a_I(\cdot)$ is required to create any required $x_{V'}$. The downside of this is the space required to store these vectors. The GIM algorithm stores the fewest interactions necessary in order to avoid any re-computations by only ever storing vectors along the current path of the search, and performing a *strict* depth first search. For example, the interaction vector $x_{\{4,3,2\}}$ is created by $a(x_{\{4,3\}}, x_2)$, where $x_{\{4,3\}}$ was just previously created in the search. Since the sub-tree under $\langle 4,2\rangle$ must have been completely examined before this is done, the vector $x_{\{4,2\}}$ is no longer in memory (it is no longer needed since $x_{\{4,2,1\}}$, for example, has already been considered). Since $x_{\{4,3\}}$ is only created and tested once the entire search space under $x_{\{4,2\}}$ has been completely examined, the search is said to be strictly depth first. As the search progresses in depth, $x_{\{4,3,2,1\}}$ is created by $a(x_{\{4,3,2\}}, x_1)$, utilising the already computed $x_{\{4,3,2\}}$. Note that one interaction expansion – where an additional variable is added to the interaction – therefore requires only one application of $a_I(\cdot)$ to create its corresponding interaction vector. Furthermore, the only interaction vectors that need to remain in memory are those on the current path of the search (due to the recursive implementation, this corresponds to the stack). Since the search is strictly depth first, there will never be a case where vectors corresponding to sibling nodes are in memory at the same time. For example, only one of $x_{\{4,1\}}, x_{\{4,2\}}, x_{\{4,3\}}$ is ever in memory at one time, even though they are siblings. There are ways to slightly reduce this space usage further; interaction vectors for sibling nodes that

are expanded last can be deleted as soon as their last child is created. For example, $\langle 4,3\rangle$ can be deleted as soon as $x_{\{4,3,2\}}$ is created (even though it is on the same path) because no other variable that has not previously been added can be added to $\{4,3\}$ without violating the order requirement of definition 3.1. For simplicity, this is not implemented here but it may be adapted from the itemset mining algorithm in chapter 4.

3.3.3 Complexity

Theorem 3.8. *The run time complexity is* $O(|I| \cdot |V| \cdot (t(m_I) + t(M_I) + t(a_I) + t(S_I) + t(I_I))$*, where* I *is the number of interactions for which* $S_I(\cdot)$ *returns true and* $t(X)$ *is the time taken to compute function* X *from the framework.*

Proof. For a node corresponding to an interaction V' to be expanded (to search for larger interactions), $S_I(\cdot)$ must return true for it and there must be siblings to join to, otherwise the branch of the search space is pruned. In the worst case, each child $V' \cup v : v \in (V - V')$ must be examined, with none of the interactions $V' \cup v$ found to be interesting according to $S_I(\cdot)$. This takes at worst $O(|V|)$ time; for each interaction mined, at worst $O(|V|)$ larger interactions may have to be examined. Finally, the processing of each interaction requires one application of each of the functions m_I, M_I, a_I, I_I and S_I. Note that $|I| \cdot |V|$ is an upper-bound on the number of interactions that must be examined. □

In most applications, $t(a_I)$ and $t(m_I)$ require at most $O(n)$ time (often less if subspaces can be exploited), since the operate on interaction vectors of at most length n and $t(M_I) = t(S_I) = t(I_I) = O(1)$. Note that if $S_I = I_I$, then the run time is linear in the number of interesting interactions found. The requirement for completeness requires that children be examined, leading to the $|V|$ in the run time. The algorithm is said to be optimal in the sense that it takes time linear in the number of patterns it finds to be interesting. Since each interaction must be generated or output, it is not possible to improve the run time beyond a constant factor. In practice, the algorithm is therefore theoretically as efficient as possible, given the frameworks functions. Of course it should be clear that $|I|$ is at worst $2^{|V|}$. In practical applications only a small proportion of these interactions are interesting however. Also, note that in the worst case, the $|V|$ component in the run time is superfluous as there exists no interaction that is not interesting – $|V|$ was included in the bound to cover interactions that were examined but not found to be interesting. Since this does not occur in the worst case, the algorithm is even optimal in the worst case. Interactions may

be output in time linear in their length, or in constant time if they are output in compressed format as a prefix tree.

If $M_I(\cdot)$ is trivial, $t(M_I) = O(1)$ and the prefix tree is never kept in memory, leading to low space usage. The effect of non-trivial $M_I(\cdot)$ is discussed in section 3.11, where the prefix tree allows compression.

Theorem 3.9. *The space usage is $O(|V| \cdot vs + |V|^2)$ if M_I is trivial, where vs is the space required by a single interaction vector.*

Proof. In the worst case (all single variables are interesting interactions), all individual variables' interaction vectors must remain in memory at one point. The search is depth first, and so the depth is at most $|V|$. At each node along the current path of the search, a list ($joinTo$) of at most size $|V|$ is kept (containing references to objects already in memory), as well as at most one additional vector (the vector corresponding to $x_{V'}$ required to build vectors for longer antecedents). Therefore, at most $O(|V| + |V|) = O(|V|)$ vectors each requiring vs space are in memory, and $O(|V|^2)$ references to existing objects already counted. □

In most applications, vs is at worst n, the number of samples. Since most databases are sparse, sparse methods can be used to simultaneously reduce the space required by interaction vectors and the run time of functions on them. Furthermore, the search can often progress in subspaces. This will be described in section 3.15. Note the order in which the x_v are used. x_v will only ever be needed by the algorithm once all possible interactions that can be created from $\{v' \in V : v' < v\}$ have been mined. This means the vector will only need to be loaded into memory at this point. Furthermore, for any variable v that is not interesting, it's vector x_v is not required. This means that the entire data set need never be in memory unless *all* single-variable interactions are interesting. It is worth highlighting the fact that there will only ever be a single interaction vector in memory at any level (depth) in the search, with the exception of depth 1 of course. This is an important advantage of the algorithm. A treatment of related algorithmic approaches and their key differences is given in section 4.3 of chapter 4.

3.4 Counting Based Approaches: The Simplest Example

In data sets where a variable is either present or absent in a sample, the simplest operation is to count how many times an interaction pattern occurs in the samples.

This can be used as the basis of of more complex methods. Frequent itemset mining (FIM) (or more generally, frequent pattern mining) is perhaps the simplest and most widespread instance of interaction mining and aims to find all sets of items in a transaction database that occur in at least *minSup* transactions [10]. A survey of such methods may be found in [43] and chapter 4 considers this problem in depth. Since FIM aims to find items that occur frequently together, it can be assumed that there is some interaction between these variables in the process generating the data; for example, an unseen variable – the human purchaser – tends to like particular combinations of items.

FIM can be implemented efficiently in the GIM framework as follows: Each item is a variable, and each transaction is a sample. The database consists of the $x_v : v \in V$ where each x_v encodes the set of transactions in which it exists. Geometrically then, items exist in the space spanned by the transaction identifiers. This idea will be covered in more detail in chapter 4. Interaction vectors $x_{V'}$ encode the set of transaction IDs whose corresponding transactions contain V'. One efficient implementation uses bit-vectors so that $x_{V'}[i]$ is 1 if the ith transaction contains V' and 0 otherwise[2]. With this encoding, $a(x_{V'}, x_v) = x_{V'}\, AND\, x_v$, the bit-wise AND operation. Since x_v encodes those transaction ids for transactions containing v, and $x_{V'}$ those containing V', $x_{V' \cup v}$ therefore encodes those transactions containing all items in V' and the item v. Note that this would be the induction step in a proof of correctness. $m_I(x_{V'}) = |x_{V'}|$, the number of set bits. Note that this is the support of the itemset V'. $M_I(\cdot)$ is trivial. Finally, $S_I(\cdot) = I_I(\cdot)$ and returns true if and only if the value computed by $m_I(x_{V'})$ is at least *minSup*. Note that the prefix tree is not kept in memory in this application since $M_I(\cdot)$ is trivial.

3.5 Mining Maximal Interactions

Interactions often overlap each other, and if an interaction is interesting then its sub-interactions are usually also interesting. In a number of applications then, only the maximal interaction is of interest. For example, this is useful in some graph mining problems and the maximal frequent itemset mining problem.

Definition 3.10. A maximal interaction $V' \subseteq V$ is an interaction for which no super-interaction V'' exists so that $V' \subset V''$ and V'' is interesting.

[2] A compressed "TID-set" or "TID-list" may also be used, which lists only the identifiers of the transactions containing V'.

Mining maximal interactions can be efficiently performed in GIM through detecting and processing "fringe" nodes.

Definition 3.11. The *fringe* of a prefix tree is the set of $PrefixNode$s that correspond to interesting interactions and are not prefixes of any other interesting interaction. Nodes in the fringe are called fringe nodes.

Note that if $S_I(\cdot) = I_I(\cdot)$ then the fringe is identical to the set of leaf nodes. Figure 3.3 shows examples of fringe nodes.

The following lemmas are useful for mining maximal interactions:

Lemma 3.12. *The set of all maximal interactions is contained in the fringe of a* $PrefixTree$.

Proof. If this were not the case, there would exist a maximal interesting interaction that were a prefix of another interesting interaction, providing a contradiction. □

It will be shown later that the GIM algorithm generates all sub-interactions $V'' \subset V'$ before generating V' (lemma 3.18). As a consequence of lemmas 3.12 and 3.18, all maximal interactions can be mined by iterating over the fringe and discarding all those interactions that are subsets of nodes mined *later* in the algorithms process. Algorithm 3.2 shows an (on-line) incremental algorithm that performs this task as the interactions are mined. Note that the subset checking must be done in one direction only thanks to lemma 3.18. Furthermore, note that a new fringe node is guaranteed to be maximal, and may only be rendered a non-maximal interaction if a *subsequently* mined interesting interaction exists that subsumes it. In algorithm 3.2, `addFringeNode(·)` is called with the fringe nodes as they are generated. These nodes are a subset of the nodes output by `outputInteraction(·)` in algorithm 3.1, and it is not difficult to modify algorithm 3.1 to be able to determine and hence provide a signal to `outputInteraction(·)` when a node is a fringe node. This can be done in constant time. Details are omitted here for clarity. Note that the maximal interactions are stored efficiently through the prefix sharing of the prefix tree.

The issues of mining maximal interactions efficiently is central to the patterns mined in chapter 9 and will be discussed in more detail there.

Algorithm 3.2 Incremental algorithm for maintaining the set of maximal interesting interactions.

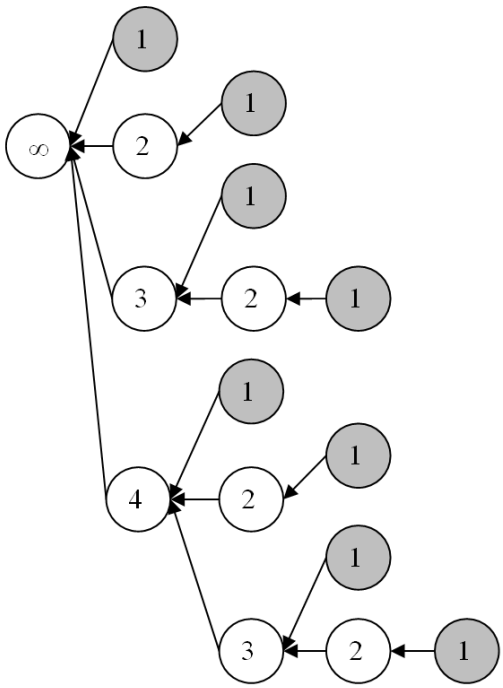
```
//Data Structure
Set maximalInteractions = ∅;

addFringeNode(PrefixNode fringeNode)
 for each PrefixNode n ∈ maximalInteractions
  if n ⊂ fringeNode
   maximalInteractions.remove(n);
 maximalInteractions.add(fringeNode);
```

3.6 Including Negative Patterns

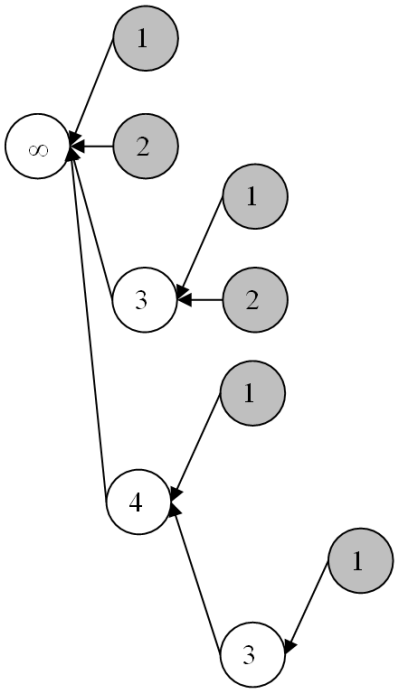
Negative patterns typically describe relationships that include the explicit *lack* of events or objects. This means that not only is an objects presence important or interesting, but so is its absence. Such patterns are (in general) *not* the same as positive and negative relationships between variables – this issue will be considered further in chapter 9. Consider an interaction pattern $P_1 = \{a, c, d\}$ where the set of variables are $V = \{a, b, c, d, e\}$ and suppose, for simplicity, that interestingness is defined by some co-occurrence measure. P_1 says that a, c and d occur together in the database. It makes no statement about the presence or absence of the other objects b and e. Indeed, b may always occur when $\{a, c, d\}$ occur, or never occur when these objects occur. If b always occurs, this leads to the pattern $P_2 = \{a, b, c, d\}$ being found. However, if it never occurs when $\{a, c, d\}$ occurs then this information is *not* found – unless negative patterns are considered. Negative patterns allows such information to be expressed; in particular, the previous example leads to the pattern $P_2 = \{a, \neg b, c, d\}$ where $\neg$ denotes the absence (negated presence). Note that P_1 and P_2 are not the same and express different knowledge about the database. Similarly, suppose that a and e *never* occur together. That is, when a is present, e is never present and vice versa. This is a potentially interesting interaction and can be expressed in two patterns $\{a, \neg e\}$ and $\{\neg a, e\}$ depending on how interesting a and e are by themselves. In contrast, not including negative patterns only allows positive interactions to be found.

Mining negative patterns can be performed by in the GIM framework by first including the negation of all variables in V. In the previous example, the variable set would then be $V = \{a, b, c, d, e, \neg a, \neg b, \neg c, \neg d, \neg e\}$. Additionally, the interaction vectors for a negated variable need to be defined. This can be done using a function:

Definition 3.13. $N : X \to X$ computes the negated vector $x_{\neg v} = N(x_v)$ corre-



(a) The fringe of the prefix tree of figure 3.2(a).



(b) Fringe of the prefix tree of figure 3.2(b)

Figure 3.3: The fringe of a prefix tree is shown in grey in this figure. Here, $S_I(\cdot) = I_I(\cdot)$ so this corresponds to the leaf nodes.

sponding to the variable $\neg v$.

Since a variable v and its negation $\neg v$ can never occur together, there is no need to consider interactions containing both. GIM can be modified to avoid examining such cases in one of two ways. The simplest way is to employ a pre-pruning function that will be described later in this chapter (definition 3.17). A more efficient method is to incorporate the categorised prefix tree introduced in chapter 6 and place each variable in a category with its negated variable. Variables in the same category are considered mutually exclusive, and this can be exploited by modifications to the algorithm that enable automatic pruning. Chapter 6 considers this in detail in the context of Generalised Rule Mining (GRM).

Note that it is not hard to avoid explicit storage of negated vectors in the actual algorithm. Usually it is easy and efficient to implement this using a *Decorator* design pattern [41] applied to the interaction vector, thus avoiding any additional usage of space.

Example 3.14. In frequent itemset mining using bit-vectors as interaction vectors, $N(\cdot)$ simple flips all bits. Note that the anti-monotonic property holds when negative items are included and as such the pruning technique functions identically to the positive item case.

Example 3.15. A real world example where negative patterns are of interest is presented in chapter 5. In that chapter, complex spatial co-location patterns were sought.

Example 3.16. In a toy example, suppose we wish to find all possible algebraic expressions with operators $-$ and $+$ over the set of variables so that the expression has a value in $[a, b]$ and holds in at least $minSup$ samples. For example, such an interaction may look like $v_1 + v_2 - v_3$, and if this is evaluated over all samples / instances in the database, and evaluates to a value in $[a, b]$ in at least $minSup$ samples, then it is an interesting pattern. This can be solved in the GIM framework using an aggregation function $a_I(x_{V'}, x_v)$ defined so that $x_{V' \cup v}[i] = x_{V'}[i] + x_v[i]$, using the variable set that includes both the positive and negated variables (where $N(x_v)[i] = -x_v[i]$), $m_I(x_{V'}) = |\{i : x_{V'}[i] \in [a, b]\}|$, $M_I(\cdot)$ is trivial, $I_I(\cdot)$ returns true if the number computed by $m_I(\cdot)$ is at least $minSup$, and $S_I(\cdot)$ always returns true (note that this means there is no pruning[3]).

3.7 Solving Top-Down or Monotonic Problems with GIM

Due to the bottom up nature of the algorithm, where interactions are grown by adding additional variables to them, GIM is most suited to methods where the interestingness measure is anti-monotonic or partially anti-monotonic, as this enables efficient pruning of the search space – particularly in sparse databases: if an interaction is not interesting, larger interactions need not be considered. This section describes how *monotonic* problems can also be solved using GIM.

It is possible to solve monotonic problems in GIM by "inverting" the original problem, thus producing an anti-monotonic problem. This means that rather than mining the interaction itself, the GIM algorithm mines the "inverted" pattern, from which the actual pattern sought can be recovered.

To illustrate this method, for simplicity consider the problem of mining *infrequent* patterns in a database where the absence of objects is meaningful. That is, find

[3] This is just a toy example, where the primary goal it to illustrate a negative pattern, not how to mine it efficiently. There are methods to solve this problem more efficiently in the GIM framework.

all sets of objects that occur *at most maxSup* times. It should be clear that this interestingness concept is monotonic. For example, if the set $\{1,2,3\}$ is interesting, then so is $\{1,2,3,4\}$ and any other super-set of $\{1,2,3\}$. Conversely, if $\{1,2,3\}$ is not interesting, then neither is $\{1,3\}$ or any other subset. This problem can be solved by starting with the interaction $\{1,2,3,4,5\}$ and *removing* variables from it. That is, a top down approach where branches of the search may be pruned accordingly. This can be achieved in GIM through inverting the problem and mining the inverted problem in a bottom up manner, therefore implicitly performing the same function as an explicitly top down algorithm. The main task is to count the occurrences of interactions in samples. That is, to count how often the pattern $\wedge_{v \in V'} v$ occurs in the rows (records, samples) $r \in D$ of the database D:

$$count(V') = |\{r \in D : v \in r\}|$$

Let us skip straight into how this can be solved in the GIM framework. Define an interaction vector $x_{V'}$ as an integer valued vector where $x_{V'}[i]$ is the number of times that *any* $v \in V'$ occurs in the ith sample. That is, $x_{V'}[i] = \sum_{v \in V'} I(v \in s_i)$ where s_i is the ith sample and $I(expr)$ has value 1 if $expr$ is true, and 0 otherwise. This may also be expressed as $x_{V'}[i] = \sum_{v \in V'} x_v[i]$ where $x_v[i]$ has value 1 if v is contained in the ith sample and 0 otherwise. Using this representation,

$$count(V') = \sum_i I(x_{V'}[i] = |V'|)$$

That is, all those entries in $x_{V'}$ are counted if they match the size of V'. The integer vector representation of these interactions allows not only the addition of variables to an interaction, but also (crucially) their removal. For example, $x_{V'-v}[i] = x_{V'}[i] - x_v[i]$. Since GIM is based on the notion of growing interactions, it is necessary to invert the problem so that adding variables using $a_I(\cdot)$ in the framework semantically corresponds to removing variables from the actual interaction being sought. This can be done using the above observations.

Therefore, the infrequent pattern mining problem can be solved in the GIM framework as follows, where $i \in [1,n]$ and n is the number of samples / rows / instances.

- $x_\infty[i] = \sum_{v \in V} x_v[i]$ is the vector corresponding to the root node (the empty interaction $V' = \emptyset$). Note however that due to the inversion of the problem, the interpretation of this node is actually the set of all variables V.
- $a_I(x_{V'}, x_v)$ is defined so that $x_{V' \cup v}[i] = x_{V'}[i] - x_v[i]$. Note that the interpre-

tation of $V' \cup v$ is actually the set of variables *except* those in $V' \cup v$. That is, $V - (V' \cup v)$. In other words, the node in the prefix tree corresponding to V' is interpreted as the interaction $V - V'$. By performing the $a_I(\cdot)$ operation, the algorithm will effectively *remove* the variable v from the interaction $V - V'$.

- $m_I(x_{V'}) = \sum_i I(x_{V'}[i] = |V| - |V'|)$, that is, the number of entries in the vector $x_{V'}$ that match the size of the desired interaction $|V| - |V'|$. Here, $I(expr)$ has value 1 if $expr$ is true, and 0 otherwise.
- $M_I(\cdot)$ is trivial, therefore simply returning the result provided by $m_I(\cdot)$.
- $S_I(\cdot) = I_I(\cdot)$ and these return true if the result of $m_I(\cdot)$ is less than or equal to $maxSup$. Note that the inversion of the problem results in an anti-monotonic interestingness measure as far as the algorithm is concerned, and therefore the search space is correctly pruned.
- $outputInteraction(PrefixNode\, node)$ in algorithm 3.1 outputs the set of variables *not* present in the traversal from *node* to the root.

It has now been shown how a monotonic problem can be inverted and mapped to an anti-monotonic problem and solved in the GIM framework. This is possible with any monotonic problem – it is simply a matter of finding the appropriate inversion.

The reader should note that this inversion is *not* related to the problem of finding negative patterns. Of course, mining positive and negative patterns with a monotonic measure is also possible using the techniques in this section.

3.8 Graph Mining: When the Input is an Adjacency or Distance Matrix

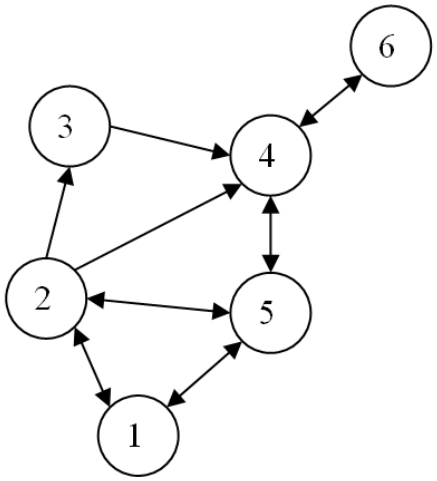
This section shows how problems can be solved in GIM that do not require measures between more than two variables at a time, however still mine interactions of any size. The result is that the input is a pre-computed adjacency matrix, which describes all pairwise interactions between variables. The task then is to use this to find larger *structural* interactions using this data. This is useful in clustering, clique mining and correlation analysis for example.

3.8.1 Clique Mining

For simplicity, consider the problem of finding all cliques in a given graph. A clique is a fully connected sub-graph (a sub-graph where every vertex is connected to every

$$A = \begin{pmatrix} 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix}$$

(a) The adjacency matrix A.



(b) Example directed graph for clique mining. It is assumed that each vertex is reachable from iteself (that is, there is an implicit edge from each vertex to itself).

Figure 3.4: Clique mining example. $a_{ij} = 1$ if there is an edge from vertex i to vertex j. $V = \{1, 2, 3, 4, 5, 6\}$. The set of cliques is $\{\{1, 2\}, \{1, 5\}, \{2, 5\}, \{4, 5\}, \{4, 6\}, \{1, 2, 5\}\}$.

other vertex, including itself). The structure of a graph may be defined by an adjacency matrix, which describes which vertexes in the graph are adjacent to which other vertexes. Specifically, the adjacency matrix A of a finite graph G on $|V|$ vertices is the $|V| \times |V|$ matrix where the non-diagonal entry a_{ij} is the number of edges from a vertex i to vertex j and the diagonal entry a_{ij}, depending on the convention, is either once of twice the number of edges from vertex i to itself. Figure 3.4 shows an example directed graph and its adjacency matrix, with the assumption that each vertex is reachable from itself.

Mining cliques can be performed in the GIM framework as follows.

- V, the set of variables, is also the set of vertices.
- The database D is the adjacency matrix, and the samples therefore are also the variables. Without loss of generality, take x_v to be the column vector, so that x_v has $x_v[i] > 0$ if the ith variable (vertex) is connected to v, and 0 otherwise. Here, vector indices start at 1.
- $a_I(x_{V'}, x_v) = x_{V' \cup v}$ where $x_{V' \cup v}[i] = \min(x_{V'}[i], x_v[i])$. Note that by this

construction, $x_{V'}[i]$ is non-zero if vertex i is connected to *all* other vertices in V'. For example, consider x_1, x_4 and x_5 from figure 3.4(a). $x_{\{1,5\}} = [1,1,0,0,1,0]^T$, showing that 1 and 5 are incident on each other, and 2 is incident on both. $x_{\{1,4\}} = [0,1,0,0,1,0]^T$, showing that 2 and 5 are both incident on 1 and 4.

If the adjacency matrix is binary, then the $x_{V'}$ are binary vectors and $a_I(\cdot)$ is the bit-wise AND operation.

- $m_I(x_{V'}) = [\sum_{v \in V'} I(x_{V'}[v] > 0), \sum_{v \notin V'} I(x_{V'}[v] > 0)]$, an array of two values where $\sum_{v \in V'} I(x_{V'}[v] > 0)$ is the number of vertices in V' that are reachable from all other vertices in V', and $\sum_{v \notin V'} I(x_{V'}[v] > 0)$ are those vertices *not* in V' that are reachable from all other vertices in V'. $I(expr)$ is the indicator variable whose value is 1 if $expr$ is true, and 0 otherwise. Note that by the construction of $x_{V'}$ by $a_I(\cdot)$, $m_I(x_{V'})[1]$ (the first value computed by $m_I(\cdot)$), this is precisely the number of vertices in V' that are connected to *all* vertices in V'. If this value is equal to $|V'|$ then V' is a clique. Note the maximum value it can take is $|V'|$.

- $M_I(\cdot)$ is trivial.

- $I_I(\cdot)$ returns true if and only if $value_m[1] = |V'|$, where $value_m$ are the values computed by $m_I(\cdot)$ and V' is the interaction being examined. Recall that if $value_m[1] < V'$ then V' is not a clique as it is not completely connected.

- $S_I(\cdot)$ returns true if and only if $value_m[1] = |V'| \wedge value_m[2] > 0$. If an interaction vector does not indicate that there are any other vertices incident on *all* vertices in V' (that is, $value_m[2] > 0$), then there is no point continuing the search by expanding V'. Therefore the search can be pruned at this point.

Note that the above approach works for both directed and undirected graphs. For a directed graph, only cliques will be mined where each vertex is connected to each other vertex so that all edges in such a clique are bi-directional. If it is known that the graph is undirected then the approach can be streamlined to make it more efficient since the adjacency matrix is symmetric. Furthermore, note that only one direction needs to be checked while the above method checks both (as it must for a directed graph).

The above method can be improved slightly. Note that given an interaction vector $x_{V'}$, it is possible to determine exactly which variables are potential candidates, and which are not. In particular $\{v \notin V' : x_{V'}[v] > 0\}$ is the set of vertices that are incident on all vertices in V'. Any vertices not in this set need not be examined and can be pruned. Note however that through the operation of GIM whereby siblings

are joined, some of this pruning is performed automatically. Furthermore, any nodes passing through this automated pruning will be discarded after one application of $a_I(\cdot)$ and $m_I(\cdot)$. That is, $O(|V|)$ time. Assuming the interaction vectors are implemented so that the $x_{V'}[v]$ look-up can be performed in $O(1)$ time, it is possible to obtain a run time improvement in cases where pruning can be applied by inserting the following line into algorithm 3.1:

```
...
for each v ∈ joinTo
  if (x_V'[v] = 0) continue; //additional line
  Vector x_V'∪v = a_I(x_V', x_v);
...
```

Where `continue` skips the remainder of the loop's current iteration. This is a small check that allows the generation and evaluation of $x_{V' \cup v}$ to be avoided. It is possible to include an additional function in the framework that generalises this and allows such efficiency improvements:

Definition 3.17. $P_I(x_{V'}, v)$ returns true if $V' \cup v$ should be examined.

With this additional function, algorithm 3.1 would look like:

```
...
for each v ∈ joinTo
  if (P_I(x_V', v)) continue; //additional line
  Vector x_V'∪v = a_I(x_V', x_v);
...
```

Finally, note that the vectors need not be implemented as an explicit vector / array. An ordered list is more space efficient and depending on the sparsity of the graph, may also be faster. A general discussion of vector representations is presented in section 3.15.

3.8.2 Mining Maximal Cliques

Maximal cliques are those cliques that are not contained inside any larger clique. Maximal cliques can be mined using GIM by using the method described in section

3.5 in addition to that described above. In figure 3.4, the maximal cliques are $\{4,5\}$, $\{4,6\}$ and $\{1,2,5\}$.

A real world example where maximal cliques are useful is presented in chapter 5. In that chapter, a specialist method for mining maximal cliques is used that functions only on two dimensional data. That is, $x_v = (x_i, y_i)$. It is not efficient for high dimensional data as it scans over the dimensions. The method described above can be used as an alternative, and is applicable to high dimensional data. Mining maximal cliques is also part of the problem considered in chapter 9.

3.8.3 Solving the Independent Set Problem

The independent set problem (ISP) is not a data mining problem, but a well known problem in algorithms. It encodes situations in which one tries to choose objects from a collection in which there are pairwise conflicts between some of the objects. The conflicts are encoded by edges between objects, which become the nodes in the graph. One wishes to find the largest set without conflicts (the largest independent set). Formally, given a graph $G = (V, E)$, a set of nodes $S \subseteq V$ is said to be independent if no two nodes in S are joined by an edge. The ISP is stated as follows: Given G, find an independent set that is as large as possible. In figure 3.4 (note that a conflict is an undirected concept), the largest independent sets are $\{6,3,5\}$ and $\{6,3,1\}$. The ISP is a general problem and subsumes problems such as interval scheduling (where the goal is to schedule a resource optimally given a set of requests) and bipartite matching. Since the ISP is NP-Complete, no efficient algorithm is known for solving it [51]. As a consequence, it is considered unlikely that an algorithm exists which can solve it more quickly that an enumeration approach.

GIM can be applied to solve the ISP problem as efficiently as can be expected by noting that ISP can be mapped to the clique mining problem above. In clique mining, sets of vertices are desired where every vertex is connected to every other, while in the ISP problem, sets of vertices are desired where none of the vertices are connected to each other. Adding a vertex that is connected to any other violates the independence property, just like adding a vertex that is not connected to all others violates the clique property. Therefore, define a graph $G^* = (V, E^*)$ where an edge exists between vertices in G^* if and only if no edge existed in G. Hence $E^* = V \times V - E$ and the adjacency matrix of G^* is the result of applying the logical NOT operation to every entry in the adjacency matrix of G. By mining a clique V' in $G*$, one is mining a set of variables V' where all variables in V' are not connected to all other variables in V'; an independent set in G. Therefore, to solve the ISP problem with GIM, V is the set of vertices and D is the adjacency matrix of G with all bits flipped so

that the column (or row) vectors x_v have $x_v[i] = 0$ if the ith variable (vertex) is in conflict with v, and 1 otherwise. Then mine cliques as described above and simply maintain only those that have the (current) largest size (note the difference between maintaining the maximal sized cliques and mining maximal cliques).

3.9 Clustering

Some clustering problems can also be solved with GIM. One example will be presented here. Consider the problem of finding all clusters so that all points in a cluster are at most $maxDist$ from their cluster center. The goal therefore is the maximal sized sets so that all points in that set are close to that set's representative point - it's center. This approach does not require the specification of the number of clusters beforehand. However, by the problem definition it can lead to overlapping clusters – that is, a point may be part of more than one cluster.

In this problem, an interaction vector $x_{V'}$ is the centroid of the cluster V'.

$$x_{V'}[i] = \frac{1}{|V'|} \sum_{v \in V'} x_v[i] \tag{3.1}$$

Note that this holds for the individual variables' interaction vectors x_v also. The search progresses by adding new points to the cluster provided that the resulting cluster center $x_{V'}$ remains within $maxDist$ from all variables in $x_{V'}$. Otherwise the search is stopped. This can be implemented in GIM as follows:

- The database is the set of vectors x_v encoding the location of the variables v in some space X. The order on V is arbitrary.
- $a_I(x_{V'}, x_v)$ is defined so that $a_I(x_{V'}, x_v)[i] = \frac{1}{|V'|+1}(|V'| \cdot x_{V'}[i] + x_v[i])$. Note that this incremental update ensures that $x_{V'}$ adheres to the result obtained by using Equation 3.1.
- It is now necessary to deviate from the exact definitions of the framework somewhat (actually, this is not necessary but it makes things clearer). Recall that $m_I(x_{V'})$ is defined as operating only on the vector $x_{V'}$. However, in this problem it is necessary to have access to the $x_v : v \in V'$ too, so that the distances can be checked. This is not a problem as these are readily accessible. $m_I(x_{V'})$ is defined as follows:

$$m_I(x_{V'}) = \max_{v \in V'} dist(x_v, x_{V'})$$

Where $dist(\cdot)$ is an appropriate distance metric. That is, the maximum distance that an element of V' is away from the cluster center $x_{V'}$.

- $M_I(\cdot)$ is trivial.
- $S_I(\cdot) = I_I(\cdot)$ and return true if and only if $m_I(x_{V'}) \leq maxDist$. If only clusters of a size at least $minClusterSize$ are required, keep $S_I(\cdot)$ as is and simply define $I_I(\cdot)$ to return true if and only if $|V'| \geq minClusterSize \wedge m_I(x_{V'}) \leq maxDist$. For example, $minClusterSize = 2$ avoids outputting any clusters of size 1.

Note that the search is pruned whenever a variable is added to the cluster that violates the condition of that cluster. Note that if this condition is violated, then adding any further variables will not change this fact, and therefore the problem is anti-monotonic. Note however that through the operation of GIM, if for example $V' = \{1, 2, 3, 4\}$ and adding a new variable 5 causes the centroid to be shifted so that 1 is no longer in the cluster, then while $\{1, 2, 3, 4, 5\}$ is not interesting, $\{2, 3, 4, 5\}$ will still be examined later and may be interesting.

Since the user will not really be interested in *all* clusters that meet the criteria above, but rather only those that are maximal, the methods of section 3.5 can be applied in order to find the desired patterns.

Finally, other cluster conditions may also be used. It is important to observe two issues however; the clustering condition should not be dependent on the order in which variables are added, unless it is permissible to have the result be dependent on the input order (Note the above method delivers the same result regardless of the order on V). Secondly, the method should have some form of anti-monotonicity (or monotonicity, in which case the approach of section 3.7 can be applied) to enable pruning. On the other hand, if a heuristic is acceptable, then this can be implemented using the $M_I(\cdot)$ function.

3.10 Mining Uncertain or Probabilistic Databases

A probabilistic database can encode uncertainty about the data. The GIM framework provides an intuitive way of solving interaction mining problems in uncertain or probabilistic databases, where the existence of variables in samples is defined by a probability vector.

In probabilistic frequent itemset mining (PFIM) for example, the goal is to find itemsets that are frequent with a high probability. In an uncertain transaction database, it may not be certain whether an item is present in a transaction. For example, noise, additive noise in privacy preserving data mining and inherent uncertainty in the problem domain may cause this to be the case. Therefore, the event "an item i is contained in a transaction t" is associated with a probability. Chapter 10 will provide more details, motivation and examples. Prior to the work presented in part IV of this thesis, all previous approaches to frequent itemset mining in uncertain and probabilistic databases used the expected support method. While this approach has many drawbacks as presented in chapter 10, it can also be implemented in GIM very efficiently. The alternative and superior method, based on computing the probability distribution of support and used in part IV, can also be implemented in GIM and this is considered in chapter 13.

The assumption made in work addressing this problem is that the items are independent, and therefore that the probability that the itemset V' exists in a transaction t_i can be computed as $\Pi_{v \in V'} P(v \in t_i)$, where $P(E)$ is the probability that event E occurs. The expected support of an itemset V' is the expected number of times it occurs in the transactions: $\frac{1}{n} \sum_i \Pi_{v \in V'} P(v \in t_i)$ where n is the number of transactions in the database. The *Expected Frequent Itemset Mining* (EFIM) problem is to search for all itemsets whose expected support is above a user defined threshold $minExpSup$. It is not hard to show that the expected support is anti-monotonic. EFIM can be solved in GIM as follows:

- The vectors x_v are defined so that $x_v[i] = P(v \in t_i)$. This results in probability vectors. The order on the variables is arbitrary.
- $a_I(x_{V'}, x_v)$ is computed as $a_I(x_{V'}, x_v)[i] = x_{V'}[i] \cdot x_v[i]$. Note that $x_{V'}[i]$ is the probability that $V' \subseteq t_i$ under the independence assumption.
- $m_I(x_{V'}) = \frac{1}{n} \sum_i x_{V'}[i]$ where n is the number of transactions. Note that this is the expectation of the support of V'.
- $M_I(\cdot)$ is trivial.
- $I_I(\cdot) = S_I(\cdot)$ and returns true if and only if $m_I(x_{V'}) \geq minExpSup$.

This problem naturally fits into the vectorised framework, which provides both an intuitive way of thinking about the problem and an efficient solution. Consider in contrast how this would be implemented using an Apriori style algorithm; in particular the need to determine whether a candidate itemset is present in a transaction.

3.11 Complex ("Non-Trivial") Interestingness Measures

So far in this chapter, all problems considered had a trivial $M_I(\cdot)$. This section will consider the case when $M_I(\cdot)$ is non-trivial. Recall from section 3.2 that this means that sub-interactions must be examined in order to calculate a measure on the interaction and to determine whether of not an interaction is interesting. This requires a way to store and quickly retrieve $PrefixNode$s given the interaction they represent, in order to obtain the $value_m$ and $value_M$ values stored within the node. This is done using a map that maps a given sequence of variables to the corresponding $PrefixNode$. Such a map is called a $SequenceMap$ and provides constant time look-up for the required values. An efficient method for implementing this is to use a Map or $Hashtable$ that maps $PrefixNode$s to themselves, with identity based solely on the sequence of variables encountered in a traversal towards the root. That is, the $hashCode()$ and equality is dependent solely on the $variableId$ sequence represented by the $PrefixNode$ and not on the values. This allows an arbitrary sequence of variables to be created (for example, as a chain of $PrefixNode$s – effectively a singly linked list), and the values of that interaction can be retrieved by retrieving the $PrefixNode$ that the algorithm created earlier via the Map's $get(\cdot)$ operation. In the worst case, this look-up operation requires $O(|V'|)$ time, where $|V'|$ is the size of the interaction (in the case of a collision, checking if two sequences are identical requires at most a scan over them).

The additional space used by this method is only the bucket array of the $HashTable$. However, recall that algorithm 3.1 assumes a garbage collector, and hence if $PrefixNode$s are not explicitly stored, they will be deleted. Storing them, as is required by a non-trivial $M_I(\cdot)$, leads to the prefix tree remaining in memory. *Conversely, note that for trivial $M_I(\cdot)$, only a single path in the prefix tree is retained in memory and furthermore, a sequence map is not required.* Insertion into this map is performed by the `store(·)` function in algorithm 3.1. Depending on the measure to be evaluated, `store(·)` may only need to store selected nodes. For example, some measures like $minPI$ and $maxPI$ require only that interactions of size 1 remain in memory for later use by $M_I(\cdot)$. In these cases, the memory requirement is the same as for a trivial $M_I(\cdot)$.

Algorithm 3.3 shows how the sequence map and the prefix tree nodes can be used to efficiently retrieve all *immediate* sub-interactions $\{V' - v : v \in V'\}$ of V'. Of course, non-immediate sub-interactions can also be retrieved.

The following lemma proves that all sub-interactions will be available, provided they are interesting. This is important for two reasons:

1. It proves correctness, and

2. It allows interestingness to be forced to be anti-monotonic simply by checking whether sub-interactions of V' exist. If they do not exist, then they are not interesting and neither can V' be if the measure is anti-monotonic. Hence, the search may be pruned at V'. This effect can be achieved by examining only immediate sub-interaction (that is, sub-interactions of size $|V'|-1$). By induction, this then holds over all sub-interactions. Forcing a measure to be anti-monotonic is a heuristic that is useful in some applications and is discussed in section 3.21.

Lemma 3.18. *Algorithm 3.1 generates all sub-interactions V'' before generating V'.*

Proof. The algorithm progresses through the search space by joining existing PrefixNode *siblings* together, creating interactions that are one variable larger than the two original sibling nodes. Suppose for the purpose of contradiction that an interaction V' exists but a sub-interaction of it is mined later. Proceed by showing that each immediate sub-interaction $V'-v : v \in V'$ has already been mined, so that the result follows by induction. First, note that each interaction can be represented by a *sequence* of PrefixNodes, which can be constructed in reverse by traversal from the node for V' towards the root. The immediate sub-interactions of V' can be obtained by removing one variable from V' at a time. Suppose $v \in V'$ is removed, so that $V' = S_p \cup v \cup S_s$ where S_p and S_s are the prefix and suffix (either potentially empty) of the interaction (sequence) respectively. Since the expansion of the search is done in depth first fashion and with increasing order amongst the siblings (according to their variables), $S_p \cup S_s$ must be expanded first, since by definition the sequences in the *PrefixTree* appear in *decreasing* order. Since this is true for all $v \in V'$, the result follows by induction and contradiction. □

3.11.1 Complexity

The run time complexity is altered only by the evaluation of $M_I(\cdot)$, as taken into account in theorem 3.8. Clearly, computing $M_I(\cdot)$ for measures that require comparison to immediate sub-interactions requires at most $O(|V|)$ extra time per interaction. Hence $t(M_I) = |V|$ at worst.

The space complexity is altered significantly, as the $PrefixNode$s must be stored in order for the algorithm to retrieve the $value_m$s of sub-interactions at a later

Algorithm 3.3 Example of an algorithm that loops through all *immediate* sub-interactions $\{V' - v : v \in V'\}$ of V' in order to compute $M_I(\cdot)$.

```
//Data Structure
Map map;

//Store
store(PrefixNode node)
 map.put(node, node);

//Function that retrieves all immediate sub-interactions of
//the interaction V' (V' is represented by node).
evaluateM_I(PrefixNode node)
 PrefixNode n = node;
 PrefixNode r; //node to temporarily remove
 PrefixNode value;
 while(n ≠ root)
  r = n;
  n = n.parent;
  if (r ≠ node)
   node.parent = n;
   value = map.get(node);
  else
   value = map.get(n);
  //value is the node representing V' − r.variableId
  //perform some computation on value.value_m and value.value_M.
  //...
  node.parent = r;
  r.parent = n;
 return the computed value.
```

stage. This means that the prefix tree over the interesting interactions must remain in memory. This is where the prefix compression of the prefix tree is valuable. Consequently, the space usage increases by exactly the number of interactions that are considered interesting according to $S_I(\cdot)$. No other space usage implications arise.

Theorem 3.19. *If $M_I(\cdot)$ requires access to sub-interactions, the space complexity is $O(|I| + |V| \cdot vs + |V|^2)$ where vs is the space required by a single interaction vector and $|I|$ is defined in theorem 3.8. Note that $O(|V| \cdot vs)$ is the worst case size of the database.*

Proof. If all interactions need to be stored ($M_R(\cdot)$ is non-trivial), this takes $O(|I|)$

space at worst as each interaction corresponds to a single prefix node. The remaining complexity is the same (see theorem 3.9). □

3.12 Weak Anti-monotonicity and when Order is Important

This fixed order in variables within the GIM framework and algorithm can be exploited. While in many applications this order is arbitrary, in some it can be used to implement a useful heuristic (for example, by expanding the most promising interactions first), while in others is can be central to the efficient mining of patterns. This section gives an example of a measure that was previously considered weakly anti-monotonic, but is actually completely anti-monotonic provided the variables are ordered in a certain fashion. Since GIM supports such an ordering, it can be used to implement weakly anti-monotonic measures very efficiently.

3.12.1 Maximum Participation Index (maxPI)

A sub-field of Data Mining concerns itself with spatial data. One problem in spatial data mining is finding co-location patterns. That is, sets of objects that are located close to each other in many instances. The *minimum participation index* , or $minPI$, is a commonly used measure in co-location mining:

$$minPI(V') = \min_{v \in V'} \{count(V')/count(\{v\})\} \tag{3.2}$$

where $count(V')$ is the number of occurrences of the interaction V' in the database. For example, $minPI$ will be used in chapter 5 for mining complex spatial co-location patterns amongst the set of all complex maximal cliques in a real world astronomy database. It is popular because it is anti-monotonic and therefore allows easy pruning of the search space: If $V" \subseteq V'$ then $minPI(V') \leq minPI(V")$. This is well known in the literature and follows readily from Equation 3.2 since support is anti-monotonic, as is the *min* function. This means that if an interaction $V"$ is found not to be interesting ($minPI$ is too low) then the search can avoid considering every super-set of V' and thus prune a large part of the search space.

An alternative to $minPI$ is the *maximum participation index* [49], or $maxPI$ measure, defined as follows:

$$maxPI(V') = \max_{v \in V'} \{count(V')/count(\{v\})\}$$

This measure is not anti-monotonic due to the max function (which by itself is monotonic) as can be demonstrated with a simple counterexample: With the addition of an extra variable v to V' so that v occurs only with the other variables in V', the ratio $count(V')/count(\{v\}) = 1$; the maximum value. Previous work has assumed that $maxPI$ is only weakly anti-monotonic [16, 49]. However it is shown here that it can be completely anti-monotonic provided the data is appropriately pre-processed. This improves the ability to use this measure to mine patterns, simplifies the algorithms and increases the efficiency of mining algorithms. It turns out that if an order is imposed on the variables, so that in the mining process only those variables are added to an existing interaction if their $count(\cdot)$ is greater than those previously added, $maxPI$ becomes anti-monotonic:

Lemma 3.20. *If* $V' = V" \cup v$ *and* $count(v) \geq \max_{j \in V"}(count(j))$ *then* $maxPI(V') \leq maxPI(V")$.

Proof. [Sketch] The numerator remains anti-monotonic, and any additional variable v added will generate a smaller ratio $count(V')/count(\{v\})$ than any existing variable $v' \in V"$. □

With this result, it is possible to use $maxPI$ anti-monotonically by ordering all variables by their $count(\cdot)$ values before engaging in the mining process. Recall that since the GIM algorithm maintains this order throughout its operation, the requirement of 3.20 is always satisfied. Hence, the correct result will be mined using GIM while the search space can be pruned as much as possible. The use of lemma 3.20 results in an $O(|V|)$ factor reduction in computation time over previous methods based on the weak anti-monotonic result.

The $maxPI$ method can be implemented anti-monotonically in the GIM framework as follows:

- Supposing we are concerned with a clique mining problem and the database consists of sub-graph instances. An interaction vector $x_{V'}$ has $x_{V'}[i] = 1$ if the ith instance in the database contains the clique V'.
- The *strict total order* $<$ is such that $v_i < v_j \iff count(v_i) > count(v_j)$. This means that variables will be added to interactions in increasing $count(\cdot)$ order,

as required to make $maxPI$ anti-monotonic. This ordering is performed as a pre-processing step.

- $a_I(\cdot)$ and $m_I(\cdot)$ are implemented as in a counting approach (see section 3.4 for example).

- $M_I(\cdot)$ can evaluate the $maxPI$ measure by using the result of $m_I(\cdot)$ (i.e. $count(V')$) and looking up the values previously computed by $m_I(\cdot)$ for individual variables (i.e. $count(v) : v \in V'$), but this is naive. Note that due to the order on the variables, it is guaranteed that $count(v) \geq \max_{j \in V''}(count(j))$, where v is the last variable added to V'. Hence $M_I(\cdot)$ need only compute $count(V')/count(v)$.

- $I_I(\cdot) = S_I(\cdot)$ and return true if and only if the result of $M_I(\cdot)$, $maxPI$, is at least a user defined threshold.

The above approach requires a *non-trivial* $M_I(\cdot)$ and an evaluation of $M_I(\cdot)$ requires $|V'|$ operations using the naive method and $O(1)$ otherwise. It turns out that there is an even more efficient implementation in GIM using a trick on the encoding of the vectors x_v. In particular, let $x_v[0]$ be $|x_v| = count(v)$. And $x_{V'}[0] = \max_{v \in V'}\{count(v)\}$. That is, the otherwise binary valued vector has an additional field storing the maximum $count(\cdot)$ of all variables in V'. The following instantiation makes this work:

- The order is as above, and so are vectors x_v except that the additional field $x_v[0]$ exists that is initiated to $count(v) = \sum_{i=1}^{n} x_v[i]$. x_∞, the vector corresponding to the root, has $x_\infty[0] = 0$ for the below to work.

- $a_I(x_{V'}, x_v)[i] = x_{V'}[i]\, AND\, x_v[i]$ when $i \geq 1$ and $\max\{x_{V'}[0], x_v[0]\}$ when $i = 0$. Note that this maintains the desired property of $x_{V' \cup v}[0]$ being the maximal $count(v') : v' \in V' \cup v$ as required.

- $m_I(x_{V'}) = |x_{V'}|/x_{V'}[0]$ where $|x_{V'}|$ is the number of set bits, that is $count(V') = \sum_{i=1}^{n} x_{V'}[i]$. $m_I(\cdot)$ therefore evaluates $maxPI$.

- $M_I(\cdot)$ is trivial. The definitions of $S_I(\cdot)$ and $I_I(\cdot)$ are as before.

This is a more efficient approach and additionally uses a trivial $M_I(\cdot)$. It also functions as an example where a clever choice for the interaction vector $x_{V'}$ leads to a more efficient algorithm.

3.13 Forced Anti-monotonicity

Work in this thesis will demonstrate that it can be desirable to force anti-monotonicity, and consequently encourages the use of this technique over selecting low quality but anti-monotonic measures. Forcing anti-monotonicity is useful when a measure exists that correlates highly with the concept of interestingness in the user's domain, but does not have any properties that can be exploited for pruning. Without searching the entire pattern space (intractable in anything but the most trivial problems) there is no way to guarantee a complete solution. An alternative is to combine the measure with a second measure that can be used for pruning, such as the number of instances that match the pattern, but then the search is determined completely by the second measure, which is usually not correlated with what the user wants. A number of concrete problems solved in this thesis demonstrate that forcing anti-monotonicity on a good interestingness measure leads to much better quality results and much more efficient algorithms than relying on measures that have natural anti-monotonicity. In particular, chapters 6, 7 and 8 use this idea for rules. This idea proved to be especially useful when mining statistically significant patterns.

Forcing anti-monotonicity generates a heuristic. Suppose we have a measure of interestingness $M(X)$ on a set X, and that higher values of $M(\cdot)$ are desirable. Anti-monotonicity means that $X \subseteq Y \implies M(X) \geq M(Y)$, therefore allowing the pruning of a search space; if X is not interesting, we need never consider any of its super-sets. The following can be used to force any non-anti-monotonic measure M' to be anti-monotonic.

Lemma 3.21. *Suppose M' is an arbitrary (not anti-monotonic) measure. The composite measure M" is anti-monotonic:*

$$M"(X) = M'(X) - \max_{x \in X}(M'(X - x))$$

Proof. By induction. □

M" is therefore the *improvement* in M' achieved by the addition of an extra variable to the interaction, since it is the difference between the interestingness of X and the most interesting immediate subset. When used in GIM, M" therefore greedily searches for new interactions that have a higher interestingness.

Implementing M" in GIM is easily achieved using the $M_I(\cdot)$ function in the framework: set $m_I(\cdot) = M'$ and have $M_I(\cdot)$ compute the equation in lemma 3.21. Recall that algorithm 3.3 showed how to access the immediate sub-interactions.

3.14 High Dimensional Data and Dimensionality Reduction

GIM is designed for high dimensional data. In particular, note from section 3.8 that it scales linearly with the dimensionality of the vectors, since the framework is based purely on vector valued functions. Since GIM operates on vectors existing in some space X, it is possible to reduce the dimensionality of those vectors without affecting the operation of GIM. Furthermore, the semantics and scrutability of the pattern do not change. That is, the results are still an interaction expressed as a subset of V. For example, the clustering approach considered in section 3.9 may easily have dimensionality reduction methods applied, since the distance measure is usually preserved quite well in the reduced space. For dimensionality reduction to be applicable in a GIM method, the result of $m_I(\cdot)$ in the reduced space should be sufficiently similar to the results when they are applied in the original space, and $a_I(\cdot)$ must lead to the same semantics in the reduced space as in the original space. Chapter 4 provides some discussion on the use of Singular Value Decomposition to reduce the space in the context of itemset mining.

3.15 Vector Representations and Subspace Projections

This section briefly discusses the importance of different vector representations in GIM and the ability for them to exploit subspace projections. Examples in this chapter have had real valued vectors (for example in section 3.6 and 3.10), integer valued vectors (for example in section 3.8 and section 3.7) and of course binary valued vectors (for example, any counting approach and some graph based approaches). Since the GIM framework operates using only functions on vectors, the way these vectors are implemented has a significant impact on the run time of these operations and hence the algorithm. Different instantiations of functions also favour different vector implementations. While it is beyond the scope of this section to give a detailed analysis, a few examples will be shown to demonstrate the issue and provide practical advice.

The most basic task in interaction mining is often determining in which samples an interaction exists. Measures on the interaction typically require only the values corresponding to these samples. First, suppose that we are interested only in the presence or absence and not the values. Then interaction vectors are (logically) sets containing those sample *id*s that contain the interaction. There are multiple ways to implement this. One method is to use a standard set implementation for $x_{V'}$.

This has the advantage that $a_I(x_{V'}, x_v)$ operates in $O(\max\{|x_{V'}|, |x_v|\})$ time (set intersection) and $m_I(x_{V'})$ operates in $O(|x_{V'}|)$ time, where $|x_{V'}|$ is the set size and is typically much less than the number of samples, n. A disadvantage is that such sets have considerable computational and space overhead. A better alternative is to use bit-vectors, where a bit $x_{V'}[i]$ is set if the ith sample contains the interaction V'. This has the advantage that $a_I(\cdot)$ is the bit-wise AND operation, which is a machine level operation and can thus be performed quickly. Also, the space usage per sample is low. Despite fast execution times and low space per sample, the runtime of $a_I(\cdot)$ and $m_I(\cdot)$ are typically $O(n)$ and space usage is $O(n)$ regardless of the logical size of the set. Another efficient method, particularly when the data is sparse, is to use an integer array storing the indexes of those samples containing V'. If this array is sorted by sample id, then intersection can be implemented very quickly and thus $a_I(x_{V'}, x_v)$ operates in $O(\max\{|x_{V'}|, |x_v|\})$ time (while still maintaining the order). $m_I(x_{V'})$ can be implemented to operate in the same time and the space usage depends on the number of non-zero values; $O(|x_{V'}|)$.

As a rule of thumb, the bit-vector approach is much faster than a set implementation. Similarly, using one bit per sample per variable uses less space in practice than a set-based implementation. The sparse method using a sorted integer array is sometimes faster than the bit-vector approach, and sometimes slower. This seems to be determined primarily by the platform used (processor and OS) and less to by the density of the vectors. The majority of the work in this thesis uses bit-vectors, as the sparse method was investigated only toward the end of the PhD.

The sparse vector method is easily extended to problems where the value of a variable or interaction is required too. For example, the problems presented in sections 3.8 and 3.7 can be expected to have sparse integer vectors and mining expected or probabilistic frequent itemsets have sparse real valued vectors. Rather than using arrays of length n, it is only necessary to store the $(index, value)$ pairs of the non-zero elements. This reduces the space required and improves the computation time of $m_I(x_{V'})$ to $O(|x_{V'}|)$, where $|x_{V'}|$ is the number of non-sparse values in the interaction vector. $a_I(x_{V'}, x_v)$ operates in $O(\max\{|x_{V'}|, |x_v|\})$. Experiments have shown that this sparse approach not only uses much less space than a full array implementation, but is also significantly faster (for example, experiments in chapter 13 demonstrate this).

3.15.1 Subspaces, Projections and Geometric Interaction Mining

Geometrically, the sparse vector method records only those dimensions (samples) spanning the subspace of X where the current interaction V' has a presence. Let

$\pi(V')$ denote this subspace. Recall that as the search progresses and the interaction is refined, additional variables are added to V' via $a_I(x_{V'}, x_v)$. Note that $V' \cup v$ exists only in the subspace formed by the intersection of the two spaces $\pi(V')$ and $\pi(v)$, since $V' \cup v$ is present only in the space where both V' and v both exist. Usually, both $\pi(V')$ and $\pi(v)$ are much smaller than the entire space X and in many cases their intersection is much smaller again. Therefore, as the search progresses the functions operate on smaller and smaller subspaces and become more and more efficient. $a_I(x_{V'}, x_v)$ can also be thought of as a projection of x_v onto the dimensions of $x_{V'}$ and vice versa. With this observation, GIM obtains a further geometric interpretation: Not only is the vectorised computational model inherently geometric, but the search progresses in terms of projections between subspaces. This observation also has a very practical consequence: each interaction vector provides an extremely fast way to find precisely the subspace containing the interaction, and hence the records / samples containing the interaction (since these records / samples span that space).

3.16 Applications and Examples in Other Chapters

This section briefly describes other problems in this thesis that have or can be solved using the GIM framework and algorithm. While the approaches described above demonstrate the breadth in the applicability of the GIM framework, the specific examples in other parts of this thesis solve problems in depth and also demonstrate the efficiency and superiority of GIM when experimentally compared to state of the art approaches for the respective problems. Performing an experimental evaluation of all the methods described above is beyond the scope of this thesis.

3.16.1 Mining Complex, Maximal and Complete Sub-graphs and Sets of Correlated Variables

Chapter 9 considers a special structural interaction capturing the complex correlation structures amongst variables. Part of the problem in chapter 9 can be solved by adapting GIM. Indeed, that problem inspired a large part of the generalised approach in this section; in particular the ability to mine maximal interactions, graphs and cliques.

3.16.2 Geometric Itemset Mining, Frequent Itemset Mining

An itemset is a particular type of interaction. Chapter 4 considers the problem of frequent itemset mining (FIM) and generalises this to interesting itemset mining, providing a geometrically inspired framework and a algorithm (GLIMIT) also based on vectors. It is shown to be faster than commonly used algorithms on the FIM problem. Again, GIM drew from the authors experience in solving that problem.

3.16.3 Mining Complex Spatial Co-location Patterns

Chapter 5 considers the problem of mining complex spatial co-locations. This problem can be solved using the GIM approach. Furthermore, the $maxPI$ method described in section 3.12.1 can now also be applied, allowing an improved interestingness measure.

3.16.4 Probabilistic Itemset Mining in Uncertain Databases

Part IV of this thesis considers the problem of mining probabilistic frequent itemsets in uncertain or probabilistic databases, including mining the probability distribution of support. One challenge is to compute the probability distribution efficiently. The other challenge is to mine probabilistic frequent itemsets using this computation. Chapter 10 uses an Apriori style algorithm for the itemset mining task. Chapter 12 introduces the first algorithm based on the FP-Growth idea that is able to handle probabilistic data. It solves the problem much faster than the Apriori style approach. Finally, chapter 13 shows how the problem can be solved in the GIM framework, leading to the GIM-PFIM algorithm. This improves the run time by orders of magnitude, reduces the space usage and also allows the problem to be viewed more naturally as a vector based problem. The vectors are real valued probability vectors and the search can benefit from subspace projections.

3.17 Conclusion

This chapter introduced the Generalised Interaction Mining (GIM) method for solving interaction mining problems at the abstract level. Since GIM leaves the semantics of the interactions, their interestingness measures and the space in which the interactions are to be mined as flexible components; it creates a layer of abstraction between a problem's definition/semantics and the algorithm used to solve it; allowing both to vary independently of each other. This was achieved by developing a consistent

but general geometric computation model based on vectors and vector valued functions. The GIM algorithm presented in this chapter can solve all problems that can be expressed in this framework. For most problems, the space required is provably linear in the size of the data set. The run-time is provably linear in the number of interactions that need to be examined. These properties allow it to outperform specialist algorithms when applied to specific interaction mining problems. This chapter demonstrated that GIM is able to solve a wide range of useful interaction mining problems – from itemset mining, to graph mining to optimisation and clustering – simply by instantiating the framework's functions in different ways. Other chapters in this thesis will consider specific interaction mining problems in depth, complete with experimental evaluations and comparisons to specialist algorithms.

Chapter 4

Geometrically Inspired Itemset Mining in the Transpose

An important interaction in data mining is the itemset pattern. In the geometric view, an itemset is a vector (*item vector*) in the space of transactions. Linear and potentially non-linear transformations can be applied to the item vectors before mining patterns. Aggregation functions and interestingness measures can be applied to the transformed vectors and pushed inside the mining process. This chapter shows that interesting itemset mining can be carried out by instantiating four abstract functions: a transformation (g), an algebraic aggregation operator ($\circ$) and measures (f and F). For *Frequent* Itemset Mining (FIM), g and F are identity transformations, $\circ$ is intersection and f is the cardinality.

Based on this geometric view, a novel algorithm is presented that uses space linear in the number of 1-itemsets to mine all interesting itemsets in a single pass over the data, with no candidate generation. It scales (roughly) linearly in running time with the number of interesting itemsets found. Experiments on the frequent itemset mining problem show that it outperforms FP-Growth on realistic data sets above a small support threshold (0.29% and 1.2% in the experiments). It always outperforms Apriori.

4.1 Introduction

Traditional Association Rule Mining (ARM) considers a set of transactions T containing items I. Each transaction $t \in T$ is a subset of the items, $t \subseteq I$. The most time-consuming task of ARM is Frequent Itemset Mining (FIM), whereby all itemsets $I' \subseteq I$ that occur in a sufficient number of transactions are generated. Specifically, if $\sigma(I') \geq minSup$, where $\sigma(I') = |\{t : I' \subseteq t\}|$ is the number of transactions containing I'. This is known as the *support* of I'.

For *item enumeration* type algorithms such as Apriori [11, 10] or FP-Growth [47], each transaction has generally been recorded as a row in the data set. These algorithms make two or more passes, reading it one transaction at a time.

In contrast, this chapter considers the data in its transposed format: Each row $x_{\{i\}}$ corresponds to an item $i \in I$ and contains the set of transaction identifiers (*tid*s) of the transactions containing i. Specifically, $x_{\{i\}} = \{t.tid : t \in T \wedge i \in t\}$. Call $x_{\{i\}}$ an *item vector* because it represents an item in the space spanned by the transactions. For simplicity, this work will use transactions and their *tid*s interchangeably when the context is clear. An example of this idea is provided in figure 4.1(a). In this example, there are 5 possible items $I = \{1, 2, 3, 4, 5\}$ and 3 transactions $T = \{t_1, t_2, t_3\}$. Since item 1 occurs in transaction t_1 and t_2, its item-vector is $\{t_1, t_2\}$. Similarly, item 2 occurs in all transactions therefore its item-vector is $\{t_1, t_2, t_3\}$. These items can be represented as vectors in the space of transactions as illustrated in figure 4.1(b), where each dimension corresponds to a transaction. Item 1 is represented by vector b, 2 by f, 3 by c and so on.

Just as an item can be represented as an item vector, so too can an *itemset* $I' \subseteq I$: $x_{I'} = \{t.tid : t \in T \wedge I' \subseteq t\}$. Figure 4.1(c) lists all itemsets that have support greater than one, and these are represented as vectors in transaction space in figure 4.1(b).

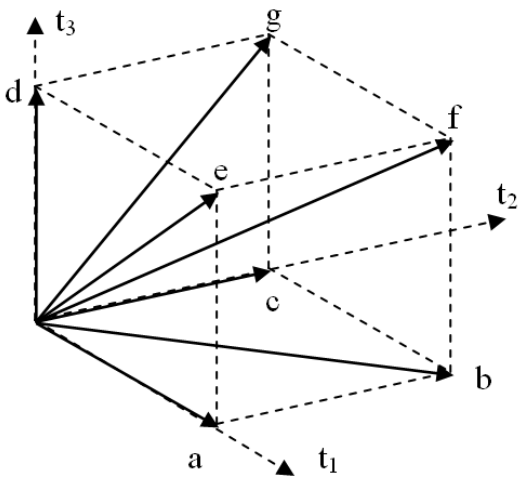
For example, consider $x_{\{4\}} = \{t_2, t_3\}$ located at g and $x_{\{2\}} = \{t_1, t_2, t_3\}$ located at f. $x_{\{2,4\}}$, the vector representing the itemset $\{2, 4\}$, can be obtained using $x_{\{2,4\}} = x_{\{2\}} \cap x_{\{4\}} = \{t_2, t_3\}$. In other words, $x_{\{2,4\}}$ is simply the vector of those transaction ids that contain both item 2 and item 4. Hence, it is located at g. It should be clear that $\sigma(I') = |x_{I'}| = |\cap_{i \in I'} x_{\{i\}}|$.

There are a three important things to note from the above:

- An item can be represented by a vector (a set representation was used above to encode its location in transaction space, but an alternate representation in some other space is equally possible).

Traditional	Transposed
$t_1 : 1, 2, 5$	$1 : t_1, t_2$
$t_2 : 1, 2, 3, 4$	$2 : t_1, t_2, t_3$
$t_3 : 2, 4, 5$	$3 : t_2$
	$4 : t_2, t_3$
	$5 : t_1, t_3$

(a) Transposing a dataset of three transactions ($tid \in \{t_1, t_2, t_3\}$) containing items $I = \{1, 2, 3, 4, 5\}$.



(b) Vectors in the space of transactions. Items and itemsets can be represented as vectors in transaction space.

label	corresponding itemsets
a	{1,5}
b	{1},{1,2}
c	{3}, {1,3}, {1,4}, {2,3}, {3,4}, {1,2,3}, {1,2,4}, {1,3,4}, {2,3,4}, {1,2,3,4}
d	{4,5}
e	{5},{2,5}
f	{2}
g	{4},{2,4}

(c) Itemsets with support greater than 1 in transaction space. Labels correspond to the vectors in figure 4.1(b).

Figure 4.1: Running item-vector example

- Item vectors can be created that represent itemsets by performing a simple operation on the item vectors (in the case above, set intersection was used).
- A measure can be evaluated using a function on the vectors (in the above case, set size was used and the measure was support). Note that only a single vector must be examined to do this.

These fundamental operations are all that are required for an itemset mining algorithm. In section 4.4 they are generalised to a function $g(\cdot)$, operator $\circ$ and function $f(\cdot)$ respectively. An additional function $F(\cdot)$ is added for more complicated measures. This generalisation allows the framework and algorithm to be applied to many other itemset mining problems, and indeed opens the door for novel approaches inspired by the geometric view that cannot be solved with existing algorithms. For example, while frequent itemset mining leads to binary values vectors, the framework could well be used for itemset mining problems that require non-binary vectors and/or measures other than support. One possible example where real vectors may be useful is the use of Singular Value Decomposition or Principle Component Analysis to reduce the dimensionality of the data set and noise prior to mining frequent itemsets. The result of such a transformation produces real valued vectors. Chapter 5 will show how the framework and algorithm presented in this chapter can be applied with a different interestingness measure in the spatio-temporal domain.

While this novel approach has many theoretical and practical benefits, it is important to note that there are a number of challenges in exploiting these ideas. The primary challenge is to compute item-vectors efficiently, and to avoid recomputing them even though they are needed at multiple points in the search. This would typically lead to a trade off between space and time. However, it turns out that this challenge can be solved using some important observations, leading to an algorithm that avoids all re-computations while maintaining minimal space usage. This challenge will be further discussed in section 4.2.

This chapter presents a single pass algorithm that uses time roughly linear in the number of interesting itemsets and at worst $n' + \lceil l/2 \rceil$ item-vectors of space, where $n' \leq n$ is the number of interesting 1-itemsets and l is the size of the largest interesting itemset. This worst case scenario is only reached with extremely low support, and most practical situations require only a small fraction of n'. Based on these facts and the geometric inspiration provided by the item-vectors, the algorithm is called *Geometrically inspired Linear Itemset Mining In the Transpose* (*GLIMIT*).

FP-Growth type algorithms are often the fastest FIM algorithms. Experiments show that GLIMIT outperforms FP-Growth [47] when the support is above a small thresh-

old. GLIMIT is more than "just another FIM/ARM algorithm" and support is just one of many possible interestingness measures it can use. It is a new, and fast, *class* of algorithm. Furthermore, it opens possibilities for useful pre-processing techniques based on the item vector framework, as well as new geometrically inspired interestingness measures.

4.1.1 Contributions

This chapter makes the following contributions:

- An interesting consequences of viewing transaction data as item vectors in transaction-space is introduced. A theoretical framework for operating on item vectors is subsequently developed. This abstraction allows a new class of algorithm to be developed, gives great flexibility in the measures used, inspires new geometric based interestingness measures and opens up the potential for useful transformations (such as pre-processing) on the data that were previously impossible.
- GLIMIT, a new, efficient and fast class of algorithm that uses the framework to mine *interesting* itemsets in one pass without candidate generation is introduced. It uses linear space and (roughly) time linear in the number of interesting itemsets. It significantly departs from existing algorithms. Experiments show it beats FP-Growth above small support thresholds when used for frequent itemset mining. It also beats Apriori.

4.1.2 Organisation

Section 4.3 places GLIMIT and the associated framework in the context of previous work. Section 4.4 presents the item-vector framework. Section 4.5.1 gives the the two data structures that can be used by GLIMIT. Section 4.5 gives the main facts exploited by GLIMIT and follows up with a comprehensive example. The space complexity is proved and pseudo-code provided. Section 4.6 shows how association rules can be mined efficiently using the output of GLIMIT. Section 4.7 presents experimental results and this chapter is concluded in section 4.8.

4.2 Some Challenges and Important Concepts

This section briefly discusses some challenges and important concepts that will aid in understanding this chapter.

4.2.1 The Transposed View

This section briefly illustrate some of the ideas used in the GLIMIT algorithm using figure 4.1(a). The goal is to convey the importance of the transpose view to the methods presented in this chapter, and introduce some of the challenges that were solved. Too keep things simple, the instantiation of $g(\cdot)$, $\circ$, $f(\cdot)$ and $F(\cdot)$ required for traditional frequent itemset mining are used. The algorithm algorithm scans the transposed data set row by row. Suppose it is scanned bottom up[1] so the first vector read is $x_{\{5\}} = \{t_1, t_3\}$. Assume $minSup = 1$. We can immediately say that $\sigma(\{5\}) = 2 \geq minSup$ and so itemset $\{5\}$ is frequent. We then read the next row, $x_{\{4\}} = \{t_2, t_3\}$, and find that $\{4\}$ is frequent. Since we now have both $x_{\{5\}}$ and $x_{\{4\}}$, we can create $x_{\{4,5\}} = x_{\{4\}} \cap x_{\{5\}} = \{t_3\}$. We have now checked all possible itemsets containing items 4 and 5. To progress, we read $x_{\{3\}} = \{t_2\}$ and find that $\{3\}$ is frequent. We can also check more itemsets: $x_{\{3,5\}} = x_{\{3\}} \cap x_{\{5\}} = \emptyset$ and $x_{\{3,4\}} = x_{\{3\}} \cap x_{\{4\}} = \{t_2\}$ so $\{3, 4\}$ is frequent. Since $\{3, 5\}$ is not frequent, neither is $\{3, 4, 5\}$ by the anti-monotonic property of support [11]. We next read $x_{\{2\}}$ and continue the process. It should be clear from the above that:

1. A single pass over the data set is sufficient to mine all frequent itemsets,
2. Having processed any $1 < j \leq |I|$ item-vectors corresponding to items in $J = \{1, ..., j\}$, it is possible to generate generate all itemsets $I' \subseteq J$ and
3. Having the data set in transpose format and using the item-vector concept allows this method to work.

4.2.2 Number of Item-vectors Used

Each item-vector could take up significant space, the algorithm may need many of them, and operations on them may be expensive. The algorithm generates at least as many item-vectors as there are frequent itemsets[2]. Since the number of itemsets is at worst $2^{|I|}-1$, clearly it is not feasible to keep all these in memory, nor is this necessary. On the other hand, it is important to avoid recomputing them as this is expensive. For example, if there are n items it is possible to use $n + 1$ item-vectors of space and create all itemsets, but this would require that most item-vectors be recomputed multiple times, leading to a vastly increased time complexity. For example, suppose

[1] This is arbitrary and simply ensures the ordering of items in the data structure used by the algorithm is increasing.

[2] It is 'at least' because some itemsets are not frequent, but it is only possible to know this once its item-vector has been calculated.

we have created $x_{\{1,2,3\}}$. When we later need $x_{\{1,2,3,4\}}$, we do not want to have to recalculate it as $x_{\{1\}} \cap x_{\{2\}} \cap x_{\{3\}} \cap x_{\{4\}}$. Instead, we would like to use the previously calculated $x_{\{1,2,3\}}$: one option is to compute $x_{\{1,2,3,4\}} = x_{\{1,2,3\}} \cap x_{\{4\}}$. The challenge is to use as little space as necessary, while avoiding *all* re-computations.

4.3 Related Work

Many itemset mining algorithms have been proposed since association rules were introduced [11, 10]. Advances can be found in [37] and [38] and a survey of frequent itemset mining can be found in [43]. Most algorithms can be broadly classified into two groups, the *item enumeration* (such as [11, 47, 74, 71, 5, 6, 73, 81, 111, 113, 72, 112]) which operate with a general-to-specific search strategy, and the *row enumeration* (such as [69, 100]) techniques which find specific itemsets first. Broadly speaking, item enumeration algorithms are most effective for data sets where $|T| >> |I|$, while row enumeration algorithms are effective for data sets where $|T| << |I|$, such as for micro-array data [69]. Furthermore, a specific to general strategy can be useful for finding maximal frequent itemsets in dense databases [88].

Item enumeration algorithms mine subsets of an itemset I' before mining the more specific itemset I'. Only those itemsets for which all (or some) subsets are frequent are generated – making use of the anti-monotonic property of support. This property is also known as the Apriori property. Apriori-like algorithms [11] search for frequent itemsets in a breadth first generate-and-test manner, where all itemsets of length k are generated before those of length $k+1$. In the candidate generation step, possibly frequent $k+1$ itemsets are generated from the already mined k-itemsets prior to counting items, making use of the Apriori property. This creates a high memory requirement, as all candidates must remain in main memory. For support counting (the test step), a pass is made over the database while checking whether the candidate itemsets occur in at least *minSup* transactions. This requires subset checking – a computationally expensive task especially when the transaction width is high. While methods such as hash-trees [88] or bitmaps have been used to accelerate this step, candidate checking remains expensive. Various improvements have been proposed to speed up aspects of Apriori. For example, [71] proposed a hash based method for candidate generation that reduces the number of candidates generated, thus saving considerable space and time. [20] argues for the use of the Trie data structure for the subset checking step, improving on the hash tree approach. Apriori style algorithms make multiple passes over the database, at least equal to the length of the longest frequent itemset, which incurs considerable I/O cost. GLIMIT does *not* perform

candidate generation or subset enumeration, and generates itemsets in a *depth first* fashion using a *single* pass over the *transposed* data set.

Frequent pattern growth (FP-Growth) type algorithms are often regarded as the fastest item enumeration algorithms. FP-Growth [47, 74] generates a compressed summary of the data set using two passes in a cross referenced tree, the FP-tree, before mining itemsets by traversing the tree and recursively projecting the database into sub-databases using conditional FP-Trees. In the first database pass, infrequent items are discarded, allowing some reduction in the database size. In the the second pass, the complete FP-Tree is built by collecting common prefixes of transactions and incrementing support counts at the nodes. at the same time, a header table and node links are maintained, which allow easy access to all nodes given an item. The mining step operates by following these node links and creating (projected) FP-Trees that are conditional on the presence of an item(set), from which the support can be obtained by a traversal of the leaves. Like GLIMIT, it does not perform any candidate generation and mines the itemsets in a depth first manner while still mining all subsets of an itemset I' before mining I'. FP-Growth is very fast at reading from the FP-tree, but the downside is that the FP-tree can become very large and is expensive to generate, so this investment does not always pay off. Further, the FP-Tree may not fit into memory. In contrast, GLIMIT uses only as much space as is required and is based on vector operations, rather than tree projections. It also uses a purely depth first search.

Many other item enumeration methods exist. [5, 6] uses a lexicographic tree and database projections in order to reduce the CPU time for counting frequent itemsets, and combine this with a depth first search. The tree is based on storing itemsets at nodes in such a way that parent nodes represent itemsets that are lexicographically before the present node. The approach uses the concept of projected transactions at nodes in the tree, observing that these projections fall in size as one descends deeper into the tree. Nevertheless, the projections must still be stored or read from disk and the frequency of lexicographic extensions counted within the projection. A matrix based method is used for support counting, requiring an additional matrix at each node. The work explores depth and breadth first methods for constructing the tree and mining frequent itemsets, as well as discussing the trade-offs that these offer.

H-Mine [73] is another projection based pattern generation approach, proposing a data structure called a H-struct to store frequent item projections of the database. The H-struct is composed of a header table for each item, and a set of hyperlinks between arrays where each array corresponds to a transaction in the current projected database. The core idea is that these hyperlinks make it easy to obtain those

transactions containing an item of interest. In many ways, this is similar to the core idea behind the conditional trees of FP-Growth. The downside of the H-struct is its potential space requirement however, as the frequent item projections and header tables must remain in memory. To overcome this, a database partitioning technique is used. Furthermore, in dense databases a hybrid approach is proposed where H-struct is combined with FP-Growth in order to take advantage of the transaction prefix sharing of FP-Trees.

Another class of item enumeration algorithm is based on the vertical approach. For example, [111] uses a vertical TID-list database format, where each item is associated with the list of transactions in which it occurs. In contrast to the traditional horizontal layout where rows are scanned, vertical methods consider columns in the database. The idea behind the vertical approach is that TID-list intersections of two itemsets X and Y give the TID-list of their union $X \cup Y$. By observing that in a lexicographic tree over the itemsets, each node corresponds not only to an itemset X but also defines an equivalence class for all itemsets with the prefix X, the search can be decomposed. This is very similar to the decomposition and database projection idea used in pattern generating approaches. Various algorithms are proposed based on different search strategies. For frequent itemset mining, Eclat is developed. It is based on a breadth or depth first traversal of the itemset lattice. The downside of this approach is that many TID-lists – in the worst case an exponential number – must remain in memory since these are required to create the TID-lists for the next level in the search.

In [112], the argument is made that vertical methods can use too much space due to the use of TID lists. To reduce this, in particular for dense data sets, the diffset is proposed. Here, it is observed that in a lexicographic tree over the itemsets, rather than storing the entire TID list for an itemset $X \cup i$, it is only necessary to store the difference in TIDs of $X \cup i$ and it's prefix X. The difference in the cardinality of these sets is the reduction in support of $X \cup i$ compared to X. Under the assumption that the database is relatively dense, this achieves a reduction in space required. Furthermore, since smaller sets are faster to intersect, this reduces the run time in such databases.

[81] presents another vertical approach, called VIPER. Viper uses a vertical TID-vector (VTV) format to represent an itemset's occurrence in transactions, encoding this in a compressed binary vector. It uses the disk to temporarily store these vectors for frequent itemsets and employs temporary horizontal tuples in counting the support of candidates. It operates in a breadth first, level wise manner; necessitating the disk based approach in order to reduce the the memory requirement.

CHARM [113] considers the closed itemset mining problem and uses a breadth or depth depth first approach in an Itemset-Tidset tree (IT-Tree). This tree is also a lexicographic tree, storing both the itemset and the TID-set at the nodes. An itemset X is closed if there exists no proper super-set $Y : X \subset Y$ such that $support(X) = support(Y)$ [72]. Closed itemsets are a loss-less way of reducing the itemsets that need to be mined while still allowing the the support of all itemsets to be calculated; for instance in the association rule discovery task. Other work on frequent closed itemsets includes [69, 74, 29, 101]. Another vertical approach is [52], where VB-FT Mine is introduced in order to mine fault tolerant frequent patterns.

[23] Introduce an efficient algorithm called MAFIA for maximal frequent pattern mining when the entire database can fit into memory, and in particular when maximal frequent itemsets are long. By using a depth first search that begins along the longest branch of a lexicographic tree, MAFIA can quickly reach the frequent itemset boundary and may thus prune away other parts of the search for maximal frequent itemsets. The approach uses the vertical layout and bitmaps instead of TID-lists.

A problem with most vertical approaches is that they keep the TID lists for sibling nodes. For example, given a node for itemset X, even when the overall search progresses in a depth first fashion (and except for maximal and closed approaches, they use a breadth first search), the child nodes and TID lists corresponding to $\{X \cup i : i \in I - X\}$ are generated and stored in memory before the search progresses in depth to one of these. This is a form of candidate generation. This is done since the fundamental operation in vertical approaches is the intersection of these TID lists. This is a significant downside, as it requires many TID lists to remain in memory. For breadth first searches, this is even worse, since the TID-lists for all frequent itemsets at the same level must me maintained – either in memory (which is not feasible in realistic databases) or on disk.

In comparison to all itemset mining algorithms, GLIMIT has most in common with vertical approaches since it also views the database column wise, by traversing the transposed database row-wise. In contrast to these vertical approaches, GLIMIT does not *store vectors for siblings at any time*. In the language of TID-lists, the intermediate TID-lists would not need to be stored in memory, except for those on the current path (of which there are at most l, where l is the length of the longest frequent itemset). Indeed, an entire sub-tree under $X \cup i$ is completely examined before $X \cup j$ is ever examined. This is termed the strict depth first search in this work. Furthermore, GLIMIT can mine all frequent itemsets in typically less space than the database (as shown in the experiments), while making only one pass over the data. Vertical approaches typically make multiple passes. While it addresses

the maximal frequent itemset mining problem (thus attempting to avoid as many frequent itemsets as possible), MAFIA [23] is perhaps the most related work to GLIMIT on the FIM problem due to the combination of a depth first search and use of bitmaps. The depth first search in MAFIA is different for two important reasons however: In MAFIA the longest branch is searched first (which aids in pruning the search for maximal frequent itemsets early), while in GLIMIT the shortest is searched first (this enables the required property that subsets are examined prior to super-sets and also allows GLIMIT to avoid loading the entire data set into memory). Secondly, child nodes are expanded before the depth is increased in MAFIA (leading to the downside mentioned above), while GLIMIT is strictly depth first. The solving of the maximal problem using various pruning techniques also requires that maximal frequent itemsets and various data structures remain in memory in MAFIA.

Row enumeration techniques effectively intersect transactions and generate super-sets of I' before mining I'. Although it is much more difficult for these algorithms to make use of the anti-monotonic property for pruning, they exploit the fact that searching the row space in data with $|T| << |I|$ becomes cheaper than searching the itemset-space. GLIMIT is similar to row enumeration algorithms since both search using the transpose of the data set. However, where row enumeration intersects transactions (rows), GLIMIT effectively intersect item-vectors (columns). But this similarity is tenuous at best. Furthermore, existing algorithms use the transpose for counting convenience rather than for any insight into the data, as is done in the framework in this chapter. Since GLIMIT searches through the itemset space, it is classified as an item enumeration technique and is suited to the same types of data. The transpose has never, to the best of the author's knowledge, been used in an item enumeration algorithm.

Efforts to create a framework for support exist. Steinbach et al. [86] present one such generalisation, but their goal is to extend support to cover continuous data. This is very different to transforming the original (non-continuous) data into a real vector-space (which is one possibility presented by the framework). Their work is geared toward existing item enumeration algorithms and so their *"pattern evaluation vector"* summarises transactions (that is, *rows*). The framework presented in this chapter operates on *columns* of the original data matrix. Furthermore, rather than generalising the support measures so as to cover more types of data sets, it generalises the operations on item-vector and the transformations on the *same* data set that can be used to enable a wide range of measures, *not* just support.

To the author's best knowledge, Ratio Rules are the closest attempt at combining SVD (or similar techniques such as Principal Component Analysis) and rule mining.

Korn et al. [53] consider transaction data where items have continuous values associated with them, such as price. A transaction is considered a point in the space spanned by the items. By performing SVD on such data sets, they observe that the axes (orthogonal basis vectors) produced define ratios between single items. The ideas in this chapter differ in a number of ways. This work considers items (*and itemsets*) in *transaction space* (not the other way around) so when SVD is considered, the new axes are linear combinations of transactions – not items. Hence I is unchanged. Secondly, this work considers mining itemsets, not just ratios between single items. Finally, SVD is just one possible instantiation of $g(\cdot)$.

As shown in this work, by considering items as vectors in transaction space, it is possible to interpret itemsets geometrically. To the author's knowledge this has not been considered previously. As well as inspiring the algorithm, this geometric view has the potential to lead to useful pre-processing techniques, such as dimensionality reduction of the transactions space. Since GLIMIT uses only this framework, it should enable the use of such techniques – which are not possible using existing FIM algorithms.

4.4 Item-vector Framework

In section 4.1, the example of frequent itemset mining (FIM) was used to introduce the ideas behind this work. However, the work in this chapter is more general than this and the instantiations of $g(\cdot)$, $\circ$ and $f(\cdot)$ are straightforward for FIM. The functions and operator formally described in this section define the form of interestingness measures and data-set transformations that are supported by the GLIMIT algorithm. Not only can existing measures be mapped to this framework, but it is the author's hope that the geometric interpretation will inspire new interesting itemset mining approaches.

Recall that $x_{I'}$ is the set of transaction identifiers of the transactions containing the itemset $I' \subseteq I$. Call X the space spanned by all possible $x_{I'}$. Specifically, $X = \mathcal{P}(\{t.tid : t \in T\})$.

Definition 4.1. $g : X \to Y$ is a transformation on the original item-vector to a different representation $y_{I'} = g(x_{I'})$ in a new space Y.

Even though $g(\cdot)$ is a transformation, it's output still 'represents' the item vector. To avoid too many terms therefore, $y_{I'}$ will also be referred to as an item vector.

Definition 4.2. $\circ$ is an operator on the transformed item-vectors so that $y_{I' \cup I"} = y_{I'} \circ y_{I"} = y_{I"} \circ y_{I'}$.

That is, $\circ$ is a commutative operator for combining item vectors to create item vectors representing larger itemsets. It is *not* required that $y_{I'} = y_{I'} \circ y_{I'}$ [3].

Definition 4.3. $f : Y \to \mathbb{R}$ is a measure on itemsets, evaluated on transformed item-vectors. Write $value_{I'} = f(y_{I'})$.

Definition 4.4. $interestingness : \mathcal{P}(I) \to \mathbb{R}$ is an interestingness measure (order) on all itemsets.

Suppose a measure of interestingness of an itemset depends only on that itemset. The simplest example is support. It is possible to represent this as follows, where $I' = \{i_1, ..., i_q\}$ and $k = 1$:

$$interestingness(I') = f(g(x_{\{i_1\}}) \circ ... \circ g(x_{\{i_q\}})) \tag{4.1}$$

So the challenge is, given an *interestingness* measure, find suitable and useful g,$\circ$ and f so that the above holds. For *support*, $\circ = \cap$, $f = |\cdot|$ and g as the identity function. Let us return to the frequent itemset mining motivation. First assume that $g(\cdot)$ trivially maps $x_{I'}$ to a binary vector. Using $x_{\{1\}} = \{t_1, t_2\}$ and $x_{\{5\}} = \{t_1, t_3\}$ from figure 4.1(a) we have $y_{\{1\}} = g(x_{\{1\}}) = 110$ and $y_{\{5\}} = g(x_{\{5\}}) = 101$. It should be clear that using bit-wise AND as $\circ$ and $f = sum()$ – the number of set bits – gives the requires semantics for frequent itemset mining.

To give a motivation for these ideas, notice that $sum(y_{\{1\}}\, AND\, y_{\{2\}}) = sum(y_{\{1\}} .* y_{\{2\}}) = y_{\{1\}} \cdot y_{\{2\}}$, the dot product (.* is the element-wise product[4]). That is, the dot product of two item-vectors is the support of the the 2-itemset. What makes this interesting is that this holds for any rotation about the origin. Suppose we have an arbitrary 3×3 matrix R defining a rotation about the origin. This means we can define $g(x) = Rx^T$ because the dot product is preserved by R (hence $g(\cdot)$). For example, $\sigma(\{1,5\}) = y_{\{1\}} \cdot y_{\{5\}} = (Rx^T_{\{1\}}) \cdot (Rx^T_{\{5\}})$. Therefore, it's possible to perform an arbitrary rotation of the item-vectors before mining itemsets of size 2. Of course

[3] Equivalently, $\circ$ *may* have the restriction that $I' \cap I" = \emptyset$.

[4] $(a. * b)[i] = a[i] * b[i]$ for all i, where [] indexes the vectors.

this is much more expensive than bit-wise AND, so why would one want to do this? Consider Singular Value Decomposition. If normalisation is skipped, it becomes a rotation about the origin, projecting the original data onto a new set of basis vectors pointing in the direction of greatest variance (incidentally, the covariance matrix calculated in SVD also defines the support of all 2-itemsets[5]). If it is also used for dimensionality reduction, it has the property that it roughly preserves the dot product. This means it should be possible to use SVD for dimensionality reduction and or noise reduction prior to mining frequent 2-itemsets without introducing too much error. The drawback is that the dot product applies only to two vectors. That is, we cannot use it for larger itemsets because the *'generalised dot product'* satisfies $sum(Rx^T_{\{1\}} .* Rx^T_{\{2\}} .* ... .* Rx^T_{\{q\}}) = sum(x_{\{1\}} .* x_{\{2\}} .* ... .* x_{\{q\}})$ only for $q = 2$. However, this does not mean that there are not other useful $\circ$, $f(\cdot)$, $F(\cdot)$ and interestingness measures that satisfy Equation 4.1 and use $g(\cdot) = SVD$, some that perhaps will be motivated by this observation.

Note that the transpose operation is crucial in applying dimensionality or noise reduction because it keeps the items intact. If the data were not transposed, the item-space would be reduced, and the results would be in terms of *linear combinations* of the original items, which cannot be interpreted meaningfully. It also makes more sense to reduce noise in the transactions than items.

Other options for $g(\cdot)$ are set compression functions or approximate techniques, such as sketches, which give estimates rather than exact values of support or other measures. However, the author believes that new *geometrically inspired* measures will be the most interesting. For example, angles between item-vectors are linked to the correlation between itemsets. Of course, it is also possible to translate existing measures into the framework.

To complete the framework, the family of functions $F(\cdot)$ is defined as follows:

Definition 4.5. $F : \mathbb{R}^{|\mathcal{P}(I')|} \to \mathbb{R}$ is a measure on an itemset I' that supports any composition of measures (provided by $f(\cdot)$) on any number of **subsets** of I'. Write $Value_{I'} = F(value_{I'_1}, value_{I'_2}, ..., value_{I'_{|\mathcal{P}(I')|}})$ where $value_{I'_i} = f(y_{I'_i})$ and all $I'_i \in \mathcal{P}(I')$.

It is now possible to support more complicated interestingness functions that require more than a measure on *one* itemset:

[5] That is, $C_M[i, j] = \sigma(\{i, j\})$.

$$interestingness(I') = F(value_{I'_1}, value_{I'_2}, ..., value_{I'_{|\mathcal{P}(I')|}}) \tag{4.2}$$

where the $value_{I'_i}$ are evaluated by $f(\cdot)$ as before.

That is, $Value_{I'} = F(\cdot)$ is evaluated over measures $value_{I'_i}$ where all $I'_i \subseteq I'$. If $F(\cdot)$ does not depend on any $value_{I'_i}$, it is left out of the notation. In that sense, call $F(\cdot)$ *trivial* if $Value_{I'} = F(value_{I'})$. In this case the function of $F(\cdot)$ can be performed by $f(\cdot)$ alone, as was the case in the examples considered before introducing $F(\cdot)$.

Example. Consider the *minPI* measure used in part for spatial co-location mining [80]: The *minPI* of an itemset $I' = \{1, ..., q\}$ is $minPI(I') = \min_i\{\sigma(I')/\sigma(\{i\})\}$. This measure is anti-monotonic and gives high value to itemsets where each member predicts the itemset with high probability. It is used in part for spatial co-location mining [80]. Using the data in figure 4.1(a), $minPI(\{1,2,3\}) = \min\{1/2, 1/3, 1/1\} = 1/3$. In terms of the framework $g(\cdot)$ is the identity function, $\circ = \cap$, $f = |\cdot|$ so that $value_{I'} = \sigma(I')$ and $Value_{I'} = F(value_{I'}, value_{\{1\}}, ..., value_{\{q\}}) = \min_i\{value_{I'}/value_{\{i\}})\}$. GLIMIT is used with *minPI* to solve a complex spatio-co-location mining problem in chapter 5.

The GLIMIT algorithm uses only the framework described above for computations on item-vectors. It also provides the arguments for the operators and functions very efficiently so it is flexible as well as fast. Because GLIMIT generates all subsets of an itemset I' before it generates the itemset I', an anti-monotonic property enables it to prune the search space. Therefore, to avoid exhaustive searches, GLIMIT generally requires[6] that the function $F(\cdot)$ be anti-monotonic in the underlying itemsets over which it operates (in conjunction with $\circ$, $g(\cdot)$ and $f(\cdot)$[7]).

Definition 4.6. $F(\cdot)$ is *anti-monotonic* if $Value_{I'} \geq Value_{I"} \iff I' \subseteq I"$, where $Value_{I'} = F(\cdot)$ is evaluated as per definition 4.5.

In the spirit this restriction, an itemset I' is considered interesting if $Value_{I'} \geq minMeasure$, a threshold. Call such itemsets *F-itemsets*.

[6] Of course, it there are few items then this constraint is not needed.
[7] Note that $f(\cdot)$ does *not* have to be anti-monotonic.

4.5 Algorithm

This section presents the GLIMIT algorithm. First, section 4.5.1 describes the required data structures. Section 4.5.2 outlines the main principles used in GLIMIT, with an illustrative example provided in section 4.5.3. The space complexity bounds are proved in section 4.5.4, followed by the algorithm in pseudo-code and a more detailed explanation of its functionality in section 4.5.5.

4.5.1 Data Structures

Prefix Tree

Recall from section 3.3.1 that a prefix tree is an efficient way to store interactions. In this chapter, a prefix tree is used to efficiently store and build frequent itemsets. It is defined a little differently here, but the approach is equivalent. An itemset $I' = \{i_1, ..., i_k\}$ is represented as a sequence $\langle i_1, ..., i_k \rangle$ by choosing a global ordering of the items (in this chapter, $i_1 < ... < i_k$). This sequence is then stored in the tree. An example of a $PrefixTree$ storing all subsets of $\{1, 2, 3\}$ is shown in figure 4.2. An example of a PrefixTree storing all subsets of $\{1, 2, 3, 4\}$ is shown in figure 4.3. Since each node represents a sequence (ordered itemset), the terms *prefix node*, *itemset* and *sequence* may be used interchangeably. The prefix tree is built of $PrefixNode$s. Each $PrefixNode$ is a tuple ($parent$, $depth$, $value$, $Value$, $item$) where $parent$ points to the parent of the node (so $n.parent$ represents the prefix of n), $depth$ is its depth of the node and therefore the length of the itemset at that node, $value$ ($Value$) is the measure(s) of the itemset evaluated by $f(\cdot)$ ($F(\cdot)$) and $item$ is the last item in the sequence represented by the node. ϵ is the empty item so that $\{\epsilon\} \cup \alpha = \alpha$ where α is an itemset. Its $PrefixNode$ (the root) is (arbitrarily) $(null, 0, NaN, NaN, \epsilon)$. To make the link with the item-vector framework clear, suppose the itemset represented at a $PrefixNode$ p is $I' = \{i_1, i_2, .., i_k\}$. Then $p.value = value_{I'} = f(g(x_{\{i_1\}}) \circ g(x_{\{i_2\}}) \circ ... \circ g(x_{\{i_k\}}))$ and $p.Value = F(\cdot)$.

The tree has the property that if a sequence s is in the PrefixTree, then so are all subsequences $s' \sqsubset s$ by the anti-monotonic property that is required of $F(\cdot)$. Note that much space is saved because the tree never duplicates prefixes. In fact, it contains exactly one node per interesting itemset.

Sequence Map

Recall from section 3.11 that a *Sequence Map* can be used to index the nodes in the $PrefixTree$ so that it is possible to efficiently retrieve them. It is used in GLIMIT

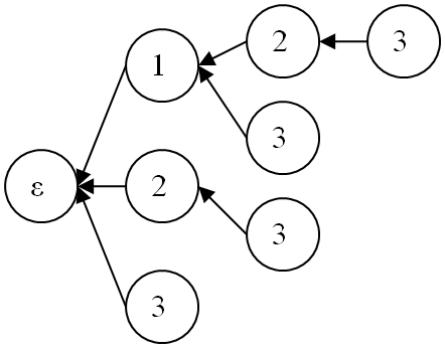


Figure 4.2: A complete prefix tree for all sub-sequences (subsets) of itemset $\{1, 2, 3\}$, where each node is labeled with *item*.

for the following purposes:

1. To check that *all* subsets of a potential itemset are interesting in order to avoid unnecessary computation of new item vectors, if this is desired. The algorithm automatically check two subsets without using the sequence map as will be shown in fact 3 in section 4.5. However, if all should be checked, the SequenceMap is required.

2. To find the the evaluated *value*s when a *non-trivial* $F(\cdot)$ must be evaluated.

3. In the FIM application, the sequence map is also used to find the evaluated support of itemsets when association rules are generated. Generating association rules will be considered in section 4.6.

4.5.2 Important Facts and Properties

The following facts are exploited in order to use minimum space while avoiding any re-computations of item-vectors.

Facts:

1. All item-vectors $y_{I'}$ can be constructed by incrementally applying the rule $y_{I' \cup \{i\}} = y_{I'} \circ y_{\{i\}}$. That is, it is only necessary to use $\circ$ to 'add' item-vectors corresponding to single items to the end of an existing item-vector. This means that given a PrefixNode p that is *not* the root, only a *single* item-vector must be kept in memory for any child of p at any point in time. If p *is* the root, it is however necessary to keep its children's item-vectors in memory (the $y_{\{i\}}$).

2. Following on from 1, this also means the least space is used if the algorithm operates in a depth first fashion. Then for any depth ($p.depth$), at most only one item-vector will be in memory at a time.

3. A new sequence is created/considered by 'joining' siblings. That is, a new sequence $\langle i_a, i_b, ..., i_i, i_j, i_k \rangle$ is considered only if siblings $\langle i_a, i_b, ..., i_i, i_j \rangle$ and $\langle i_a, i_b, ..., i_i, i_k \rangle$, $k > j$ are in the prefix tree. Hence, only those nodes are expanded that have one or more siblings *below* it. This is an exploitation of the anti-monotonic requirements of $F(\cdot)$.

4. Suppose the items are $I = \{i_1, i_2, ..., i_n\}$. If the algorithm has read in k item-vectors $y_{\{i_j\}}$ $j \in \{n, n-1, .., n-k-1\}$, then it is possible to have completed all nodes corresponding to all subsets of $\{i_{n-k-1}, ..., i_n\}$. Therefore, if a depth first procedure is used, when a PrefixNode p is created all PrefixNodes corresponding to subsets of p's itemset will already have been generated. As well as being the most space efficient approach, this is required to evaluate nontrivial $F(\cdot)$. In this chapter, this is called the 'bottom up' order of building the Prefix Tree.

5. When a PrefixNode p with $p.depth > 1$ (or $p.item$ is the top-most item) cannot have any children (because it has no siblings by fact 3), its item-vector will no longer be needed.

6. When a topmost *sibling* (the topmost *child* of a node) is created (or it is found that its itemset is not interesting – e.g. not frequent – and hence don't need to create it), the item-vector corresponding to its *parent* p can be deleted. That is, the algorithm has just created the topmost (last) immediate child of p. This applies only when $p.depth > 1$ or when $p.item$ is the top-most *item*[8]. This is because $y_{\{i_a,i_b,...,i_i,i_j\}}$ is only needed until $y_{\{i_a,i_b,...,i_i,i_j,i_k\}} = y_{\{i_a,i_b,...,i_i,i_j\}} \circ y_{\{i_k\}}$ is generated where $i_a < i_b <, ..., < i_i < i_j < i_k$ (e.g.: $b - a$ and a may both greater then 1, etc) and $\{i_a, i_b, ..., i_i, i_q\} : j < q < k$ is not interesting (e.g. not frequent). Indeed, the algorithm may write the result of $y_{\{i_a,i_b,...,i_j\}} \circ y_{\{i_k\}}$ directly into the item-vector holding $y_{\{i_a,i_b,...,i_j\}}$. Conversely, while there is still a child to create (or test) it is not possible to delete p's corresponding item-vector.

7. When a PrefixNode p is created on the topmost *branch* (e.g.: when all itemsets are frequent, p will correspond to $\langle i_1, i_2, .., i_k \rangle$ for any $k \geq 1$), the algorithm can delete the item-vector corresponding to the single item $p.item$ (e.g.: i_k).

[8] By fact 1 it is not possible to apply this to nodes with $p.depth = 1$ (unless it is the topmost node) as they correspond to single items and are still needed for later expansion.

Fact 6 will always apply in this case too (e.g.: the algorithm can also delete i_{k-1} if $k > 1$). The reason behind this is that by using the bottom up method (and the fact that itemsets are ordered), it is known that if the algorithm has created $y_{\{i_1,\ldots,i_k\}}$ then it can only ever $\circ$ a $y_{\{i_j\}}$ with $j > k$ onto the end.

4.5.3 Algorithm Example

This section presents an example of how the algorithm operates on the frequent itemset mining problem in order to illustrate some of the facts and properties presented in section 4.5.2.

Suppose we have the items $\{1, 2, 3, 4\}$ and the *minMeasure* (in this case *minSup*) threshold is such that all itemsets are considered frequent. Figure 4.3 shows the target prefix tree and figures 4.4 and 4.5 show the steps performed in mining it. This example serves to show how the algorithm manages the memory while avoiding any re-computations of item-vectors. For now, consider the frontier list in the figure as a list of PrefixNodes that have not been completed. The frontier will be discussed in the next section to avoid complicating this example. It should be clear that a bottom up and depth first procedure is used to mine the itemsets, as motivated by facts 2 and 4. The algorithm completes all sub-trees before moving to the next item. In figure 4.4(c) $y_{\{3,4\}} = y_{\{3\}} \circ y_{\{4\}}$ is calculated as per fact 1. Note fact 3 is also used – $\{3\}$ and $\{4\}$ are siblings. Once the node for $\{3, 4\}$ has been created in figure 4.4(c), the algorithm can delete $y_{\{3,4\}}$by fact 5. It has no possible children because of the ordering of the sequences. The same holds for $\{2, 4\}$ in figure 4.4(e). In figure 4.4(f), the node for $\{2, 3\}$ is the topmost sibling (child). Hence fact 6 can be applied in figure 4.4(g). Note that by fact 1, the algorithm calculates $y_{\{2,3,4\}}$ as $y_{\{2,3,4\}} = y_{\{2,3\}} \circ y_{\{4\}}$. Note also that because the algorithm needs the item-vectors of the single items in memory it has not been able to use fact 7 yet. Similarly, fact 6 is also applied in figure 4.5(b), (c), (e) and (f). However, note that in (c), (e) and (f) the algorithm also uses fact 7 to delete $y_{\{2\}}$, $y_{\{3\}}$, and $y_{\{4\}}$. In figure 4.5(b) $y_{\{1\}}$ was deleted for two reasons: Fact 6 and 7 (it is a special case in fact 6). Finally, to better illustrate fact 3, suppose $\{2, 4\}$ is not frequent. This means that $\{2, 3\}$ will have no siblings anymore. This means the algorithm does not even consider $\{2, 3, 4\}$ by fact 3.

4.5.4 Algorithm Complexity

The time complexity is roughly linear in the number of frequent itemsets because all re-computations of item-vectors are avoided. Recall that a possible downside of

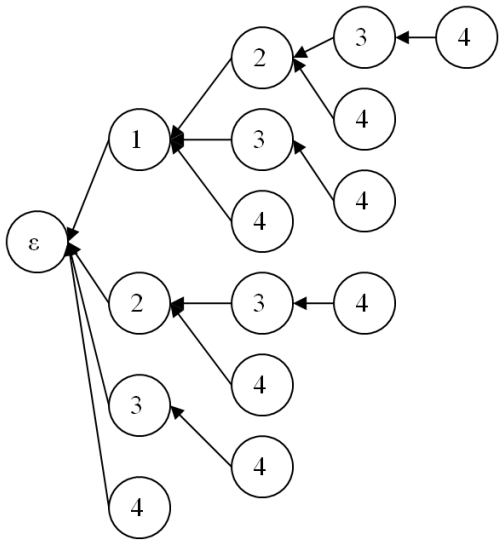
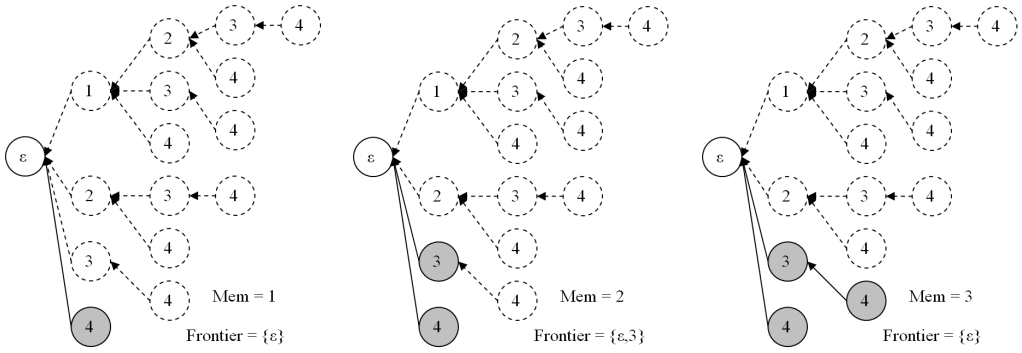


Figure 4.3: Complete prefix tree (when all itemsets are interesting).

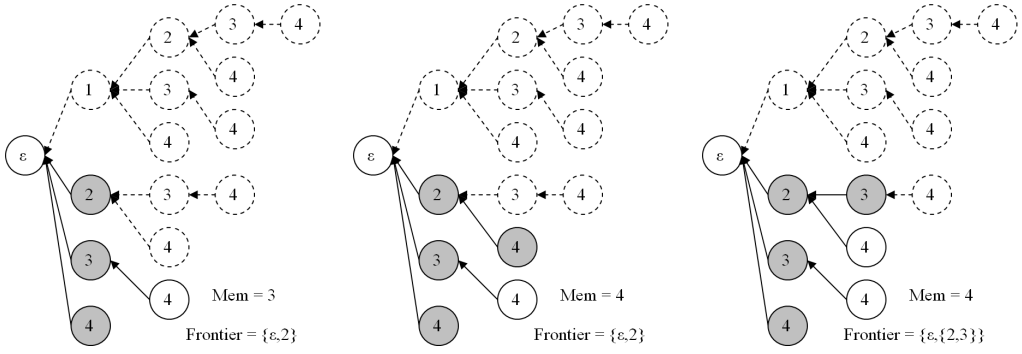
this is that the space usage could increase. The primary question therefore is; what is the maximum number of item-vectors that the algorithm may have in memory at any time?

There are two main factors that influence this.

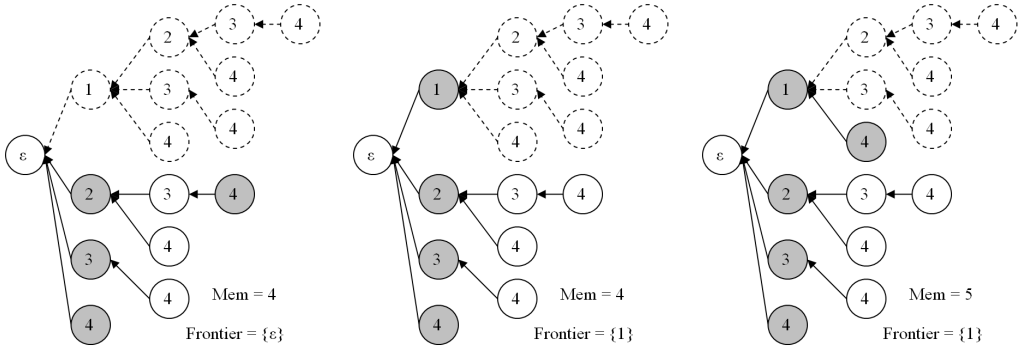
- First, the algorithm must keep the item-vectors for individual items in memory until it has completed the node for the top-most item (fact 1 and 7). Hence, the 'higher' up in the tree the algorithm is, the more this contributes to space usage.
- Secondly, the algorithm must keep item-vectors in memory until it completes their respective nodes. That is, check all their children (fact 6) or if they can't have children (fact 5). Now, the further we are up in the tree (or any sub-tree for that matter) without completing the node, the longer the sequence of incomplete nodes is and hence the the more item-vectors need to be kept. Considering both these factors leads to the situation in figure 4.6 – that is, the algorithm is up to the top item and the topmost path from that item so that no node along the path is completed. As before, solid lines are parts of the tree that have been created, dotted lines are for parts that are still to be examined, and shaded nodes are nodes with an item-vector in memory. If there are n items, the worst case item-vector usage is just the number of coloured nodes in figure 4.6. There are n item-vectors $y_{\{i\}} : i \in \{1, ..., n\}$ corresponding to the single items (children of the root). There are a further $\lceil n/2 \rceil$ item-vectors



(a) Step 1 (b) Step 2 (c) Step 3

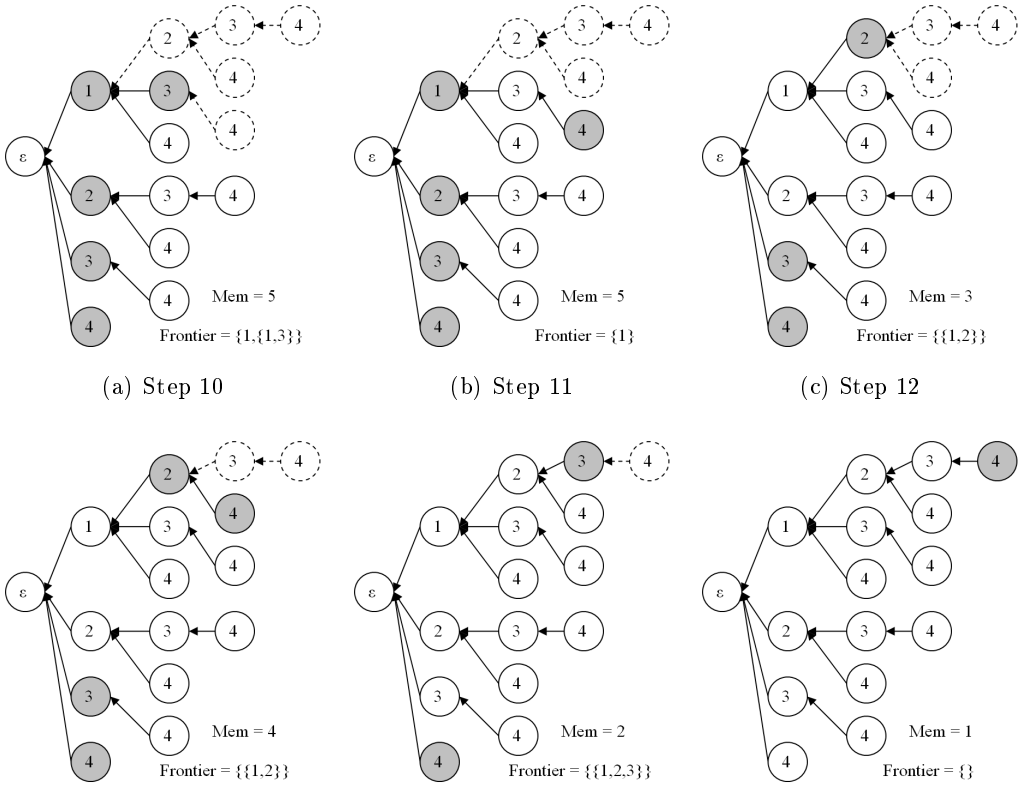


(d) Step 4 (e) Step 5 (f) Step 6



(g) Step 7 (h) Step 8 (i) Step 9

Figure 4.4: Mining example. Nodes are labeled with their *item* value. Shaded nodes have their corresponding item-vector in memory. Dotted nodes have not been mined yet. Solid lines are the parts of the tree that have been created. Continued in Figure 4.5.



(a) Step 10 (b) Step 11 (c) Step 12

(d) Step 13 (e) Step 14 (f) Step 15

Figure 4.5: Mining Example. Continuation of figure 4.4.

along the path from node $\{1\}$ (inclusive) to the last coloured node (these are the uncompleted nodes). When n is even, the last node is $\{1,3,5,...,n-3,n-1\}$ and when n is odd it is $\{1,3,5,...,n-2,n\}$. The cardinality of both these sets, equal to the number of nodes along the path, is $\lceil n/2 \rceil$. Note that in the even case, the next step to that shown will use the same memory (the item-vector for node $\{1,3,5,...,n-3,n-1\}$ is no longer needed once $\{1,3,5,...,n-3,n-1,n\}$ is created by by fact 6, and the algorithm writes $y_{\{1,3,5,...,n-3,n-1,n\}}$ directly into $y_{\{1,3,5,...,n-3,n-1\}}$ as it is computed so both need never be in memory at the same time). Therefore the total space required is just $n + \lceil n/2 \rceil - 1$, where the -1 is so that the item-vector for $\{1\}$ is not double counted.

The above discussion considers the worst case when all itemsets are frequent. Clearly, a closer bound can be obtained if $n' \leq n$ is the number of frequent items. Hence, the algorithm requires space linear in the number of frequent items. The multiplicative constant (1.5) is low, and in practice (with non-pathological support thresholds), the algorithm uses far fewer than n item-vectors or space. That is, less than the size of

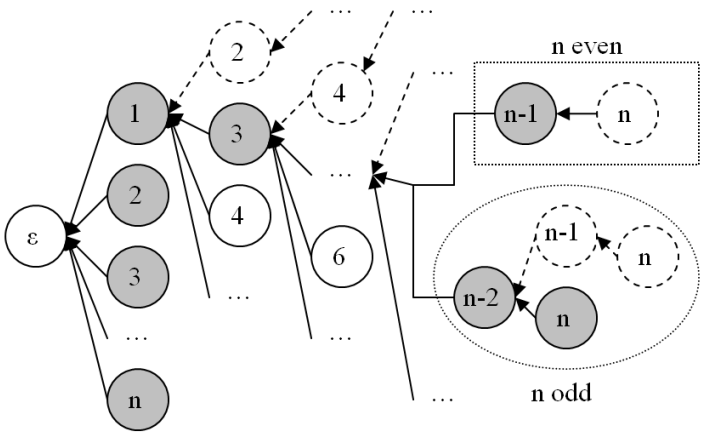


Figure 4.6: Maximum number of item-vectors needed. There are two cases: n odd (nodes in the oval) and n even (nodes in the rectangle).

the data set itself. Supposing we know that the longest frequent itemset has size l, then it is additionally possible to bound the space by $n' + \lceil l/2 \rceil - 1$. Furthermore, since the frontier contains all uncompleted nodes, the above implies that its upper bound is $\lceil l/2 \rceil$. The previous discussion is a proof sketch of the following lemma:

Lemma 4.7. *Let n be the number of items, and $n' \leq n$ be the number of frequent items. Let $l \leq n'$ be the largest itemset. GLIMIT uses at most $n' + \lceil l/2 \rceil - 1$ item-vectors of space. Furthermore, $|frontier| \leq \lceil l/2 \rceil$.*

4.5.5 Algorithm Details

The algorithm is a depth first traversal through the search space, thus building the $PrefixTree$ in a depth first manner. The search is implemented using the *frontier* method, whereby a list (priority queue) of states (each containing a node that has yet to be completely expanded) is maintained. The general construct is to retrieve the first state, evaluate it for the search criteria, expand it (create some child nodes), and add states corresponding to the child nodes to the frontier. The frontier contains any nodes that have not yet been completed, wrapped in *State* objects. Algorithm 4.1 describes the additional types used (such as *State*) and shows the initialisation and the main loop – which calls $step(\cdot)$. It also describes the $check(\cdot)$ and $calculateF(\cdot)$ methods, used by $step(\cdot)$.

Algorithm 4.1 describes the additional types used (such as *State*), shows the initialisation and the main loop – which calls the primary procedure $step(\cdot)$ in algorithm 4.2. It also shows the $check(\cdot)$ and $calculateF(\cdot)$ methods, used by algorithm 4.2.

The pseudo-code is java-like, a garbage collector is assumed which simplifies it, indentation defines blocks and type casts are ignored.

Let α be the itemset of length k represented at node *node* (assuming *node* is not the root). *node.item* is the last element of α. The *check*(*node*, *item*) method in algorithm 4.1 checks whether $\alpha \cup \{item\}$ can be frequent – in the sense that all its subsets have already been found to be frequent. This is true if and only if all subsets of size k are frequent. Note that it is already known that α and $(\alpha - \{node.item()\}) \cup \{item\}$ (the itemset of the sibling of *node*) are frequent. Hence the method must just check the other $\begin{pmatrix} k+1 \\ k \end{pmatrix} - 2$ subsets. It does this by first traversing from *node* back toward the root to obtain the itemset, and then looking up the subsets in the SequenceMap to see if the corresponding PrefixNode exists. By the bottom up construction, all the required subsets have already been generated and added to the SequenceMap (HashTree) using *hashtree.add*(*node*). It should be noted that the correctness does not depend on *check*() being called. Indeed, *check*() can do nothing and the correct results will still be delivered. This decision is a trade off between checking if subsets exist or calculating the vectors for new sets. In other words, it is a heuristic.

It has been explicitly shown when extra item-vectors are required (allocated) and when they are deleted through the use of the global variable $totalMem$ that tracks the amount of item-vectors of space needed. Note that the algorithm prepares $buffer$ for all the subsequent calls to *step*($\cdot$). Normally (when $it.hasNext()$), $buffer$ cannot be modified by the receiving method as it is required again for subsequent calls. However, then it has progressed to the 'top' of the list of siblings ($it.hasNext() = false$), the receiving method *can* modify $buffer$ – and will effectively 'steal' the item-vectors from it to reuse (reducing the size of $buffer$). From then on it will be responsible for decrementing $totalMem$ when these 'stolen' item-vectors are no longer used. This explains the last line of the algorithm.

Finally, a few minor points: If *node* is the root, the algorithm is has not been called from itself and so has not already put the item-vectors over which *it* iterates in memory. Hence the memory required to read from file must be counted. Also, *it.remove*() is ignored if the Iterator is reading from file.

4.6 Mining Association Rules

This section describes how association rules can be generated very efficiently. Algorithm 4.3 presents the method, and the following lemma describes it and proves its

Algorithm 4.1 Data types, initialisation, main loop and auxiliary methods. The primary processing is done in algorithm 4.2.
Input:
(1) A data set (in *inputFile*) in transpose format (*may* have $g(\cdot)$ already applied)
(2) $f(\cdot)$, $\circ$, $F(\cdot)$ and $minMeasure$.
Output: Completed $PrefixTree$ ($prefixTree$) and $SequenceMap$ (map) containing all *F-itemsets*.

Data Types:

$Pair$: ($Itemvector\, y_i$, $Item\, item$)
//y_i is the item-vector for $item$ and corresponds to y_i in fact 1.
//They are reused through $buffer$:
$State$: ($PrefixNode\, node$, $Itemvector\, y_{I'}$, $Iterator\, itemvectors$, $boolean\, top$, $Pair\, newPair$, $List\, buffer$)
//$y_{I'}$ is the item-vector corresponding to $node$ (and $y_{I'}$ in fact 1).
//$buffer$ is used to create the *Iterators* (such as $itemvectors$) for the *States*
//created to hold the children of $node$. $buffer$ is needed to make use of fact 3.
// $itemvectors$ provides the y_i to join with $y_{I'}$ and $newPair$ helps in doing this.

Initialisation:

initialise $prefixTree$ with its root. Initialise map and $frontier$ as empty.
//Create initial state:
$Iterator\, itemvectors = new\, AnnotatedItemvetorIterator(inputFile)$;
//Iterator is over $Pair$ objects and reads input one row at a time and annotates
//the item-vector with the item it corresponds to. Could also apply $g(\cdot)$
$frontier.add(new\, State(prefixTree.getRoot(), null, itemvectors, false, null, new\, LinkedList()))$;

Main Loop:

while (!$frontier.isEmpty()$)
  $step(frontier.getFirst())$; //See algorithm 4.2

Auxiliary Methods:

/*Let α be the itemset corresponding to $node$. $\alpha \cup \{item\}$ is the itemset represented by a child p of $node$ so that $p.item = item$. $value$ would be $p.value$. This method calculates $p.Value$ by using map to look up the $PrefixNode$s corresponding to the k required subsets of $\alpha \cup \{item\}$ to get their $value$ values, $value_1, ..., value_k$. Then it returns $F(value_1, ..., value_k)$.*/
$double$ **calculateF**($PrefixNode\, node, Item\, item, double\, value$)
//details depend on $F(\cdot)$

/*Check whether the itemset $\alpha \cup \{item\}$ could be interesting by exploiting the anti-monotonic property of $F(\cdot)$: use map to check whether subsets of $\alpha \cup \{item\}$ (except α and $(\alpha - node.item) \cup \{item\}$ by fact 3) exist.*/
$boolean$ **check**($PrefixNode\, node, Item\, item$)
//details omitted

Algorithm 4.2 Procedure to perform one expansion. *state.node* is the parent of the new $PrefixNode$ ($newNode$) that we create if $newNode.Value \geq minMeasure$. $localTop$ is true iff we are processing the top sibling of *any* sub-tree. $nextTop$ becomes $newNode.top$ and is set so that top is true only for a node that is along the *topmost branch* of the prefix tree.

void **step**(*State state*)
  if ($state.newPair \neq null$) //see end of method ♣
    $state.buffer.add(state.newPair)$;
    $state.newPair = null$; //so it won't be added again
  $Pair\, p = state.itemvectors.next()$;
  $boolean\, localTop$ =!$state.itemvectors.hasNext()$;
  if ($localTop$)
    //Remove *state* from $frontier$ (and hence delete $state.y_{I'}$) as the
    //the top child of *node* is being created in this step. Fact 6
    $localFrontier.removeFirst()$;
  $Itemvector\, y_{I'\cup\{i\}} = null$; $double\, value, Value$;
  $boolean\, nextTop$; //top in the next *State* we create.
  if ($state.node.isRoot()$) //we are dealing with itemsets of length 1 (so $I' = \{\epsilon\}$)
    $value = f(p.y_i)$; $Value = calculateF(null, \{p.item\}, value)$; $y_{I'\cup\{i\}} = p.y_i$;
    $state.top = localTop$; $nextTop = localTop$; //initialise *top*s.
  else
    $nextTop = localTop$ && $state.top$;
    if ($check(state.node, p.item)$) //make use of pruning property
      if ($localTop$ && ($state.node.getDepth() > 1$ || $state.top$)) //Fact 6 or 7
        //No longer need $state.y_{I'}$ as this is the last child we can create under
        //*state.node* (and it is not a single item other than perhaps the topmost)
        $y_{I'\cup\{i\}} = state.y_{I'}$;
        $y_{I'\cup\{i\}}\circ = p.y_i$; //can write result directly into $y_{I'\cup\{i\}}$
      else //need to use additional memory for the child ($y_{I'\cup\{i\}}$).
        $y_{I'\cup\{i\}} = state.y_{I'} \circ p.y_i$;
      $value = f(y_{I'\cup\{i\}})$; $Value = calculateF(state.node, \{p.item\}, value)$;
    else //don't need to calculate since it is known that $Value < minMeasure$
      $value = Value = -\infty$
  if ($Value \geq minMeasure$) //Found an interesting itemset - create $newNode$ for it.
    $PrefixNode\, newNode = prefixTree.createChildUnder(state.node)$;
    $newNode.item = p.item$; $newNode.value = value$; $newNode.Value = Value$;
    $sequenceMap.put(newNode)$;
    if ($state.buffer.size() > 0$) //there is potential to expand $newNode$. Fact 5
      $State\, newState = new\, State(newNode, y_{I'\cup\{i\}}, state.buffer.iterator()$,
        $nextTop, new\, LinkedList())$;
      //add to front of frontier so depth first search. Fact 2.
      $frontier.addFront(newState)$; $state.newPair = p$;
      //if *state.node* is not complete, p will be added to $state.buffer$ *after*
      // $newState$ has been completed. See ♣

correctness.

Lemma 4.8. *Let $s = \langle i_1, ..., i_k \rangle = \alpha\beta\gamma$ be the sequence corresponding to a prefix node n where $\alpha, \beta \neq \emptyset$. All association rules can be generated by creating all rules $\alpha \Rightarrow \beta$ and $\beta \Rightarrow \alpha$ for each leaf node in the prefix tree.*

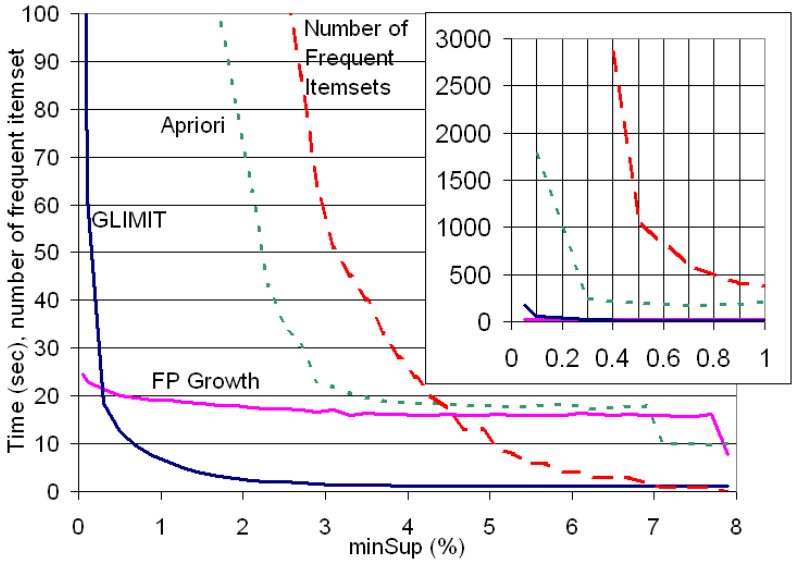
Proof. (Sketch) Given a leaf node n corresponding to a sequence $s =< i_1, ..., i_k >$, algorithm 4.3 generates all the rules $\alpha \Rightarrow \beta$ and $\beta \Rightarrow \alpha$ for all α, β, γ where $\alpha \neq \emptyset$ is a prefix of s, γ is a possibly empty suffix of s, and $\beta \neq \emptyset$ is the remaining sub-string (a suffix iff $\gamma = \emptyset$). That is, $s = \alpha\beta\gamma$. It is not possible to generate all possible association rules that can be generated from itemset $\{i_1, ..., i_k\}$ by considering only node n. Specifically, the following are missed: (1) any rules $\alpha' \Rightarrow \beta'$ or $\beta' \Rightarrow \alpha'$ where α' is not a prefix of s, and (2) any such rules where there is a gap between α' and β'. However, by the construction of the tree there exists another node n' corresponding to the sequence $s' = \langle \alpha', \beta' \rangle$ (since $s' \sqsubset s$). If n' is not in the fringe, then by definition $s' \sqsubset s$" where s" $= \langle \alpha', \beta', \gamma' \rangle$ for some $\gamma' \neq \emptyset$ and n" (the node for s") is in the fringe. Hence $\alpha' \Rightarrow \beta'$ and $\beta' \Rightarrow \alpha'$ will be generated from node(s) other than n. Finally, the longest sequences are guaranteed to be in the fringe, hence all rules will be generated (and without duplication) by induction. □

In this procedure, the evaluated measures ($value$, $Value$) for α are stored in the prefix nodes visited by the algorithm as α is a prefix of s. To obtain the evaluated measures for β, the PrefixNode (βn) corresponding to β must be obtained. This is done using a *Sequence Map* (map) that has also been built by the mining algorithm.

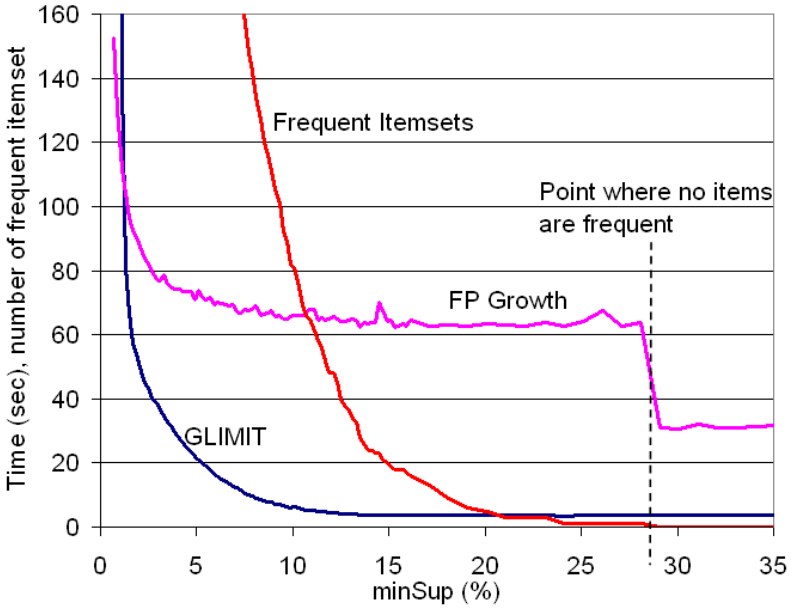
4.7 Experiments

The GLIMIT algorithm was evaluated on two publicly available data sets from the FIMI repository[9] – T10I4D100K and T40I10D100K. These data sets have 100,000 transactions and a realistic skewed histogram of items. They have 870 and 942 items respectively. To apply GLIMIT, the data was first transposed as a pre-processing step. This is cheap, especially for sparse matrices – precisely what the data sets in question typically are. The data used was in the experiments was transposed in 8 and 15 seconds respectively using a naive Java implementation and without exploiting sparse techniques.

[9] http://fimi.cs.helsinki.fi/data/

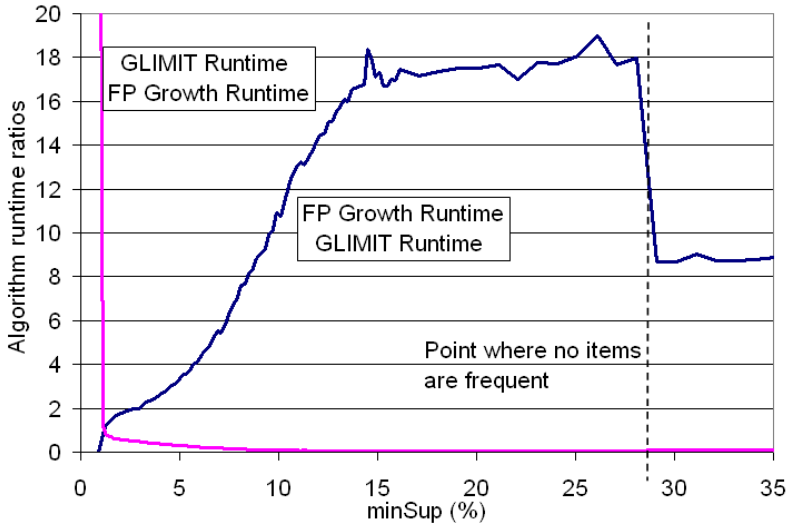


(a) Runtime and frequent itemsets. T10I4D100K. Inset shows detail for low support.

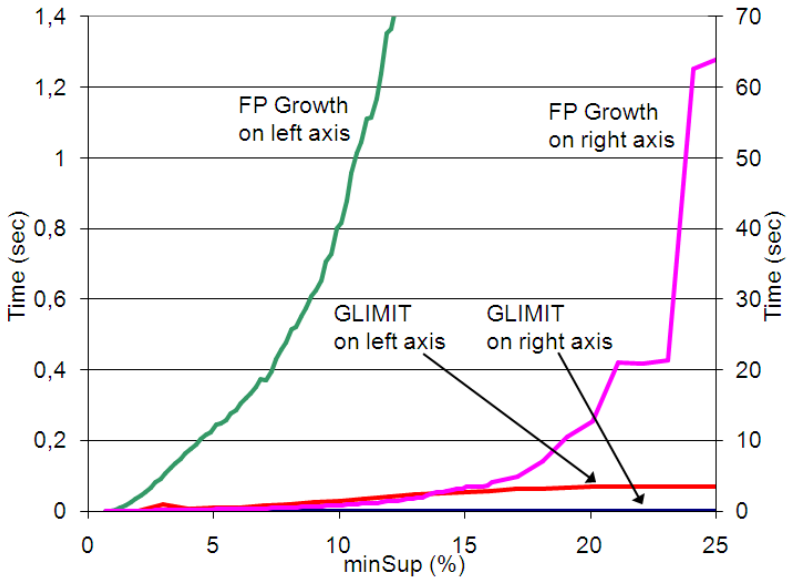


(b) Runtime and frequent itemsets. T40I10D100K.

Figure 4.7: Run time results. Apriori, FP-Growth and GLIMIT.



(a) Runtime ratios. T10I4D100K.



(b) Average time taken per frequent itemset shown on two scales. T10I4D100K.

Figure 4.8: Run time results. FP-Growth and GLIMIT.

Algorithm 4.3 Generating association rules from the prefix tree. This should be called for each PrefixNode in the fringe to output all rules. We assume the measure is support and we evaluate for confidence.

void **generateAssociations**($PrefixNode\ fringeNode$)
  for ($PrefixNode\ \alpha\beta n = fringeNode$; $\alpha\beta n.item \neq \epsilon$; $\alpha\beta n = \alpha\beta n.parent$)
    $\sigma_{\alpha\cup\beta} = \alpha\beta n.M$; $\beta size = 1$;
    for ($PrefixNode\ \alpha n = \alpha\beta n.parent()$; $\alpha n.item \neq \epsilon$; $\alpha n = \alpha n.parent$)
      $Sequence\ \beta seq = \alpha\beta n.getSuffix(\beta size++)$;
      $PrefixNode\ \beta n = map.get(\beta seq)$;
      $\sigma_\alpha = \alpha n.Value$; $\sigma_\beta = \beta n.Value$;
      $c_{\alpha\Rightarrow\beta} = \frac{\sigma_{\alpha\cup\beta}}{\sigma_\alpha}$; $c_{\beta\Rightarrow\alpha} = \frac{\sigma_{\alpha\cup\beta}}{\sigma_\beta}$;
      /*output the rules and their σ and cs*/
      output(αn, βn, $\sigma_{\alpha\cup\beta}$, $c_{\alpha\Rightarrow\beta}$);
      output(βn, αn, $\sigma_{\alpha\cup\beta}$, $c_{\beta\Rightarrow\alpha}$);

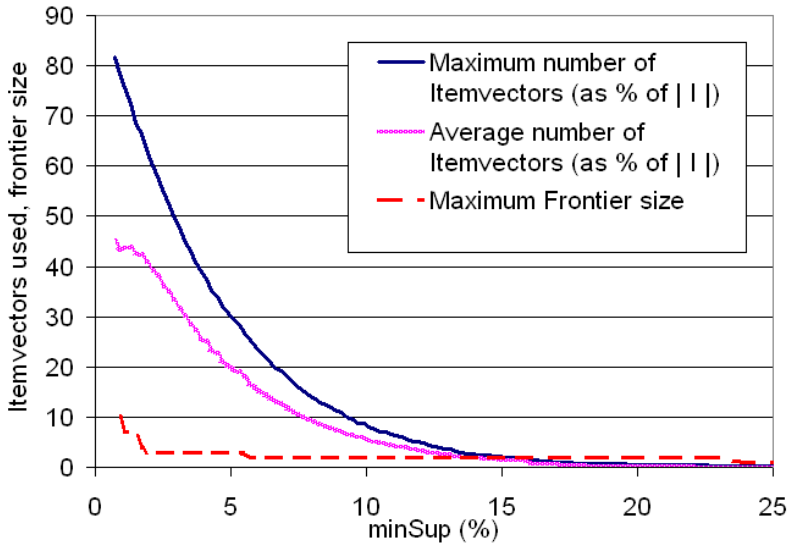


Figure 4.9: Number of item-vectors needed and maximum frontier size. Data set: T10I4D100K.

GLIMIT was compared to a publicly available implementation of FP-Growth and Apriori. The algorithms used were from ARtool[10] as it is also written in Java and has been available for some time. The algorithms were not used via the supplied GUI, but rather the underlying classes were invoked directly to avoid overheads.

The primary goal of this section is to show that GLIMIT is fast and efficient when compared to existing algorithms on the traditional FIM problem. Recall that a major contribution of this chapter however is the item-vector framework that allows operations that previously could not be considered, and a flexible and new class of algorithm that uses this framework to efficiently mine data cast into different and useful spaces. The fact that it is also very fast when applied to traditional FIM is a consequence of this. To represent item-vectors for traditional FIM, bit-vectors were used[11] so that each bit is set if the corresponding transaction contains the item(set). Therefore g creates the bit-vector, $\circ = AND$, $f(\cdot) = sum(\cdot)$ and $F(m) = m$.

Figure 4.7(a) shows the run time[12] of FP-Growth, GLIMIT and Apriori[13] on T10I4D100K, as well as the number of frequent items. The analogous graph for T40I10D100K is shown in figure 4.7(b). Apriori was not run in this experiment as it is too slow. These graphs clearly show that when the support threshold is below a small value (about 0.29% and 1.2% for the respective data sets), FP-Growth is superior to GLIMIT. However, above this threshold GLIMIT outperforms FP-Growth significantly. Figure 4.8(a) shows this more explicitly by presenting the run time ratios for T40I10D100K. FP-Growth takes at worst 19 times as long as GLIMIT. These results indicate that GLIMIT is superior above a threshold. Furthermore, this threshold is very small and practical applications usually mine with much larger thresholds than these.

GLIMIT scales roughly linearly in the number of frequent itemsets. Figure 4.8(b) demonstrates this experimentally by showing the average time to mine a single frequent itemset. The value for GLIMIT is quite stable, rising slowly toward the end (as in these cases GLIMIT must still check itemsets, but very few of them turn out to be frequent). FP-Growth on the other hand, clearly does not scale linearly. The reason behind these differences is that FP-Growth first builds an FP-tree. This effectively stores the entire Data set (minus infrequent single items) in memory. The FP-tree is also highly cross-referenced so that searches are fast. The downside is that this takes significant time and a lot of space. This pays off extremely well when the support threshold is very low, as the frequent itemsets can read from the tree very

[10] http://www.cs.umb.edu/ laur/ARtool/.
[11] The *Colt* (http://dsd.lbl.gov/~hoschek/colt/) BitVector implementation was used.
[12] Pentium 4, 2.4GHz with 1GB RAM running WindowsXP Pro.
[13] Apriori was not run for extremely low support as it took longer than 30 minutes for $minSup \leq 0.1\%$

quickly. However, when *minSup* is larger, much of the time and space is wasted. GLIMIT uses time and space as needed, so it does not waste as many resources, making it fast. The downside is that the operations on bit-vectors (in our experiments, of length $100,000$) can be time consuming when compared to the search on the FP-tree, which is why GLIMIT cannot keep up when *minSup* is very small. Figure 4.9 shows the maximum and average[14] number of item vectors our algorithm uses as a percentage of the number of items. At worst, this can be interpreted as the percentage of the data set in memory. Although the worst case space is 1.5 times the number of items, n (lemma 4.7), the figure clearly shows this is never reached in these experiments. The maximum was approximately $0.82n$. By the time it were to get close to $1.5n$, *minSup* would be so small that the run time would be unfeasibly large anyhow. Furthermore, the space required drops quite quickly as *minSup* is increased (and hence the number of frequent items decreases). Figure 4.9 also shows that the maximum frontier size is very small. (recall from lemma 4.7 it is bounded above by $\lceil l/2 \rceil$. Finally, recall that the algorithm can avoid using the prefix tree and sequence map on the FIM problem, so the only space required are the item vectors and the $frontier$. That is, the space required is truly linear.

4.8 Conclusion and Future Work

This chapter showed interesting consequences of viewing transaction data as item-vectors in transaction-space and developed a framework for operating on item-vectors. This abstraction gives great flexibility in the measures used and opens up the potential for useful transformations on the data. Future work may involve finding useful geometric measures and transformations for itemset mining. One particular problem of interest is to find a way to use SVD prior to mining for itemsets larger than 2. This chapter also presented GLIMIT, a novel algorithm that uses the framework and significantly departs from existing algorithms. GLIMIT mines itemsets in one pass without candidate generation, in linear space and time linear in the number of interesting itemsets. Experiments showed that it beats FP-Growth above small support thresholds and is always faster than Apriori.

[14] over the calls to $step(\cdot)$.

Chapter 5

Fast Mining of Complex Spatial Co-location Patterns

Most algorithms for mining interesting spatial co-locations integrate the co-location / clique generation task with the interesting pattern mining task and are usually based on the Apriori algorithm. This has two downsides: First, it makes it difficult to meaningfully include certain types of complex relationships – especially *negative* relationships – in the patterns. Secondly, the Apriori algorithm is slow.

This work mines complex co-location relationships between object types; a special type of interaction between variables. It considers maximal cliques of galaxies in an astronomy dataset which are used to extract complex maximal cliques. These are subsequently mined for interesting sets of object (galaxy) *types,* including complex types such as absence and multiple occurences. It is shown that the GLIMIT itemset mining algorithm can be applied to this problem, leading to far superior performance than using an Apriori style approach.

The problem may be solved directly using the GIM framework.

5.1 Introduction

A spatial data set often describes *Geo-spatial* or *"Astro-spatial"* (astronomy related) data. In this work, a large astronomical data-set containing the location of different *types* of galaxies is used [1]. Data sets of this nature are very large and provide many opportunities and challenges for data mining applications. The use of novel data mining approaches has the potential to uncover interesting patterns and knowledge in such data sets.

One such pattern is the *co-location* pattern. A co-location pattern describes a group of objects (such as galaxies) where each object is located in the neighborhood (within a given distance) of another object in that group.

A *clique* is a special type of co-location pattern. A clique is a group of objects such that *all* objects in that group are co-located with each other. In other words, given a predefined distance, if a group of objects lie within this distance from every other object in the group, they form a clique. Figure 5.1 shows 8 different objects $\{A1, A2, A3, B1, B2, B3, B4, C1\}$, with lines between them indicating that they are co-located. The set $\{B1, B2, A3\}$ is a clique. However, $\{B1, B2, A3, C1\}$ is not, because $C1$ is not co-located with $B2$ and $A3$. Similarly, $\{B1, B2, A3, C1\}$ is a co-location pattern but it is not a clique.

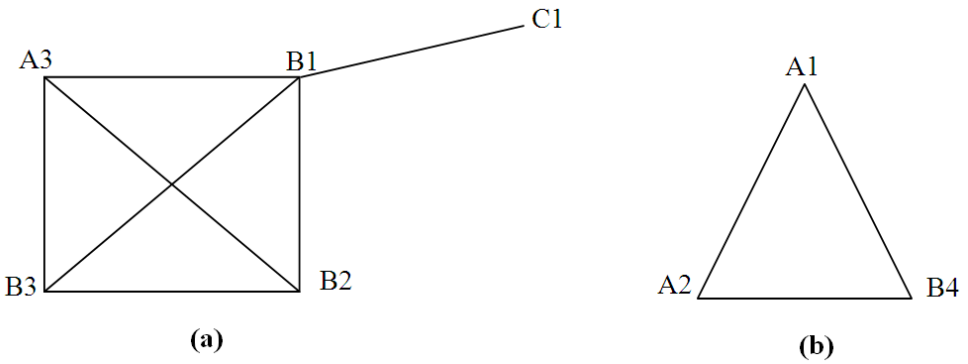


Figure 5.1: Clique example.

This work considers *maximal cliques*. A maximal clique is a clique that does not appear as subset of another clique in the same co-location pattern (and therefore the entire data set, as each object is unique). For example, in Figure 5.1, $\{A1, A2, B4\}$ forms a maximal clique as it is not a subset of any other clique. However, $\{A3, B2, B3\}$ is not a maximal clique since it is a subset of the clique $\{A3, B1, B2, B3\}$ (which in turn *is* a maximal clique). The second column of Table 5.1 shows all the maximal cliques in Figure 5.1.

ID	Maximal Cliques	Raw Maximal Cliques	Non-Complex Relation-ships	Complex Without Negative Re-lationships	Complex With Negative Re-lationships
1	{A3, B1, B2, B3}	{A, B, B, B}	{A, B}	{A, B, B+}	{A, B, B+, -C}
2	{B1, C1}	{B, C}	{B, C}	{B, C}	{-A, B, C}
3	{A1, A2, B}	{A, A, B}	{A, B}	{A, A+, B}	{A, A+, B, -C}

Table 5.1: Representing maximal cliques of Figure 5.1 as complex relationships

In the data set used in this work, each row corresponds to an object (galaxy) and contains its type as well as its location. The goal is to mine relationships between the *types* of objects. Examples of object types in this data set are "early-type" galaxies and "late-type" galaxies. To clarify; of interest are not co-locations of *specific* objects, but rather, co-locations of object types *types*. Finding complex relationships between such types is useful information in the astronomy domain. In Figure 5.1, there are three types: $\{A, B, C\}$. This Chapter focuses on using maximal cliques in order to allow mining of interesting *complex spatial relationships* between the object types.

A *complex spatial relationship* includes not only whether an object type, say A, is present in a (maximal) clique, but also:

- Whether *more than one* object of its type is present in the (maximal) clique. This is called a *positive type* and is denoted by $A+$.
- Whether objects of a particular type are not present in a *maximal clique* – that is, the absence of types. This is called a *negative type* and is denoted by $-A$.

The inclusion of *positive* and / or *negative types* makes a relationship *complex*. This allows mining patterns that indicate, for example, that A occurs with multiple B's but not with a C. That is, the presence of A may imply the presence of multiple object of type B and the absence of objects of type C. This is interesting in the astronomy domain as it show complex relationships between different types of galaxies. The last two columns of Table 5.1 show examples of (maximal) complex relationships.

This work is not concerned with *maximal* complex patterns (relationships) by themselves, as they provide only local information; that is, local information about a particular maximal clique. Rather, this work is concerned with *sets* of object types (including complex types), that appear across the entire data set – that is, amongst

many maximal cliques. In other words, the goal is to find *interesting complex spatial relationships* (sets), where "interesting" is defined by a global measure. Returning to the astronomy data set, this means patterns will be found showing complex relationships between galaxy types that reoccur throughout the data set.

The global measure of interestingness used in this work is a variation of the $minPI$ [80] measure:

$$minPI(P) = \min_{t \in P}\{N(P)/N(\{t\})\} \tag{5.1}$$

Here, P is a set of complex types being evaluated and $N(\cdot)$ is the number of maximal cliques that contain the set of complex types. Note that the occurrences of the pattern (set of complex types) are counted only in the maximal cliques. This means that if the $minPI$ of a pattern is above α, then it is possible to say that whenever any type $t \in P$ occurs in a maximal clique, the entire pattern P will occur in at least a fraction *alpha* of those maximal cliques. $minPI$ is superior to simply using $N(P)$ because it scales by the occurrences of the individual object types, thus reducing the impact of a non-uniform distribution on the object types. This is important, as otherwise those object types that occur frequently dominate the results.

This work focuses on *maximal cliques* for the following reasons:

- The process of forming complex positive relationships only makes sense in maximal cliques. Suppose we extract a clique that is not maximal, such as $\{A1, B4\}$ from Figure 5.1. We would not generate the positive relationship $\{A+, B\}$ from this, even though each of $\{A1, B4\}$ are co-located with $\{A2\}$. The correct pattern emerges only once maximal cliques are considered.

- Negative relationships are possible. For example, consider the maximal clique in row 1 of Table 5.1. If *maximal* cliques were not used, then we would also consider $\{B1, B2, B3\}$, and from this we would *incorrectly* infer that the complex relationship $\{B, B+, -A\}$ exists. However, this is not true because A *is* co-located with each of $\{B1, B2, B3\}$. *Therefore, using non-maximal cliques will generate incorrect* negative patterns because negative types cannot be inferred until the maximum clique is mined.

- Each maximal clique will be considered as a single instance (transaction) for the purposes of counting. In other words, using maximal cliques automatically avoids counting the same objects within a maximal clique multiple times.

- Using maximal cliques reduces the total number of cliques by removing all redundancy. So not only does this lead to better quality results as outlined above, but it also reduces the computational cost of the subsequent mining process. Furthermore, since it is possible to mine maximal cliques directly without first considering all sub-cliques, this leads to a further computational advantage.

5.1.1 Problem Statement

Problem Statement: Given the set of maximal cliques, find all interesting and complex patterns that occur amongst that set of maximal cliques. More specifically, find all *sets* of object types, including *positive* and *negative* (complex) types that have a $minPI$ above a user defined threshold.

It will be shown that this problem can be mapped to an *itemset mining* task with $minPI$ used as an interestingness measure. In order to solve it very quickly, the GLIMIT algorithm of Chapter 4 is applied, as will be described in Section 5.5.

Including negative types makes the problem much more difficult, as it is typical for spatial data to be sparse. This means that the absence of a type amongst maximal cliques is very common. This is analogous to having a very large transaction width in frequent itemset mining, which is known to be very challenging for mining algorithms. In contrast to standard approaches relying on an Apriori style algorithm that find this very difficult, it will be shown that this is not a problem for the approach described in this Chapter.

5.1.2 Contributions

This Chapter makes the following contributions:

- It introduces *maximal cliques* and describes how they make more sense than simply using cliques in co-location mining. Furthermore, it is shown that they allow the use of negative patterns.
- A general and modular Knowledge Discovery in Databases (KDD) process is introduced that splits the maximal clique generation, complex pattern extraction and interesting pattern mining tasks into independent components.
- It shows that GLIMIT can be used to mine complex, interesting co-location patterns very efficiently in very large real world data sets. Indeed, it is demon-

strated that GLIMIT can be almost three orders of magnitude faster than using an Apriori based approach.

5.1.3 Organisation

The rest of this Chapter is organized as follows: Section 5.2 describes the complete KDD process for mining complex spatial co-location patterns. Section 5.3 formally defines maximal cliques. Section 5.4 defines complex relationships and shows how these are extracted. Section 5.5 describes how the complex spatial co-location mining problem can be considered as an itemset mining problem, while Section 5.5.1 shows how it can be mapped to the GLIMIT framework and hence solved using the GLIMIT algorithm. Section 5.6 shows how it can be solved using the GIM. Section 5.7 presents experiments and an analysis of the results. Section 5.8 places the contributions in context of related work and this Chapter is concluded in Section 5.9.

5.2 Complex Spatial Co-location Pattern Discovery Process

Figure 5.2 shows the overall flowchart of the method described in the Chapter. First, a maximal clique mining algorithm finds all *maximal cliques* and strips them of the object identifiers. This produces raw maximal cliques as shown in Table 5.1. One pass is then made over the raw maximal cliques in order to extract complex relationships, as will be described in Section 5.4. This produces maximal complex

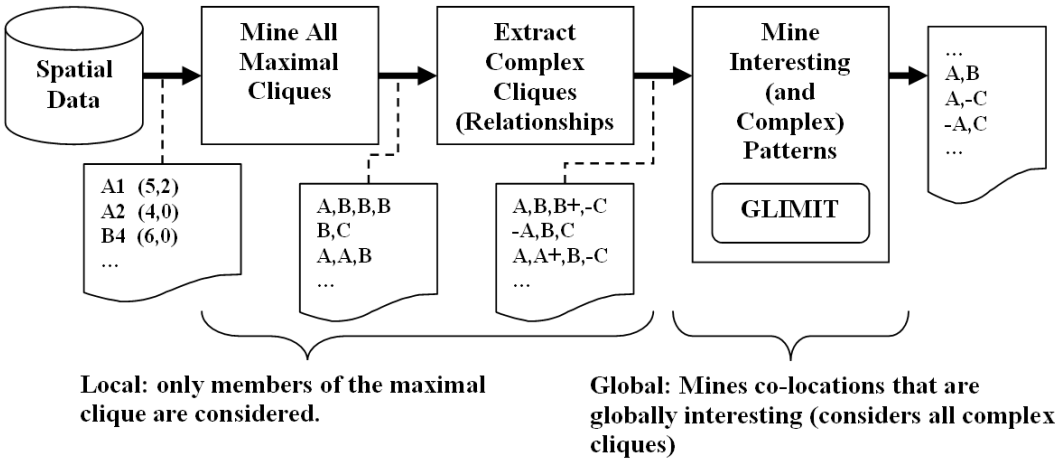


Figure 5.2: The complete mining process.

cliques. Each of these complex, maximal cliques is then considered as a *transaction*, and an *interesting itemset mining algorithm*, using *minPI* as the interestingness measure, is used to extract the interesting complex relationships. This is described in Sections 5.5 and 5.5.1.

As shown in Figure 5.2, the clique generation and complex relationship extraction are local procedures, in the sense that they deal only with individual maximal cliques. In contrast, the interesting pattern mining is global – it finds patterns that occur across the entire space. Secondly, subsets of maximal cliques are only considered in the last step – that is, after the complex patterns have been extracted.

5.3 Maximal Cliques

Consider a set of objects O with fixed locations. Given an appropriate distance measure $d : O \times O \rightarrow \mathbb{R}$, define a graph G as follows; let O be the set of vertices and construct an edge between two objects $o_1 \in O$ and $o_2 \in O$ if $d(o_1, o_2) \leq \tau$, where τ is a chosen distance.

Definition 5.1. A *co-location pattern* is a connected sub graph in G.

Definition 5.2. A *clique* $C \in O$ is any fully connected sub graph of G. That is, $d(o_1, o_2) \leq \tau \; \forall \{o_1, o_2\} \in C \times C$.

As was mentioned in Section 5.1, maximal cliques are used in this work so that complex patterns can be meaningfully defined and used, and to avoid double counting which would heavily skew the results towards large cliques.

Definition 5.3. A *maximal clique* C_M is a clique that is not a subset (sub-graph) of any other clique.

The mining of maximal cliques is done directly – it does *not* require mining all sub-cliques first in an enumeration style approach. The maximal clique mining algorithm is described in [12].

5.4 Extracting Complex Relationships

A relationship is called complex if it consists of *complex types* as defined in Section 5.1.

Extracting a complex relationship R from a maximal clique C_M involves using the following rules for every type t:

1. If C_M contains an object with type t, $R = R \cup t$.
2. If C_M contains more than one object of type t, $R = R \cup t+$.
3. If C_M does not contain an object of type t, $R = R \cup -t$.

Note that if R includes a positive type $A+$, it will also *always* include the basic type A. This is necessary so that maximal cliques that contain $A+$ will also be counted as containing A when they are mined for interesting patterns. Recall that the negative type only makes sense if *maximal cliques* are used. The last three columns of Table 5.1 show the result of applying Rule 1, Rule 1 and then Rule 2, and all three rules, respectively.

5.5 Mining Interesting Complex Relationships

The complex relationships considered in this chapter are specific types of interactions between variables, and hence can be solved using the GIM framework and algorithm. At the time this work was performed, GIM had not been developed. Instead, the problem is mapped to itemset mining. Solving the problem directly in GIM is described in section 5.6.

In *itemset mining*, the data set consists of a set of transactions T, where each transaction $t \in T$ is a subset of a set of *items* I; that is, $t \subseteq I$. In order to map complex spatial co-location mining to the itemset mining task, the set of complex maximal cliques (relationships) become the set of transactions T. The items are the object types – including the complex types such as $A+$ and $-A$. For example, if the object types are $\{A, B, C\}$, and each of these types is present and absent in at least one maximal clique, then $I = \{A, A+, -A, B, B+, -B\}$. An interesting itemset mining algorithm mines T for interesting itemsets. The support of an itemset $I' \subseteq I$ is the number of transactions containing the itemset: $support(I') = |\{t \in T : I' \subseteq t\}|$. So called *frequent itemset mining* uses the support as the measure of interestingness. For reasons described in Section 5.1, this work uses *minPI* (see Equation 5.1) which, under the mapping described above, is equivalent to

$$minPI(I') = \min_{i \in I'} \{support(I')/support(\{i\})\} \tag{5.2}$$

Since $minPI$ is *anti-monotonic*, the search space for interesting patterns can easily be pruned.

5.5.1 Mapping the Problem to GLIMIT

Recall from Chapter 4 that GLIMIT is a fast and efficient itemset mining algorithm that has been shown to outperform Apriori [11] and FP-Growth [47]. Since it is based on a framework of functions (Section 4.4), new measures can easily be incorporated. In particular, the $minPI$ measure can be build on top of the frequent itemset mining approach: Recall from example 4.4 on page 79 that it can be incorporated into GLIMIT as follows (let $I' = \{1, 2, ..., q\}$ for simplicity): $g(\cdot)$ is the identity function (there is no transformation on the data set), $\circ = \cap$ (intersection) and $f(\cdot) = |\cdot|$ (the set size). Let $m_{I'}$ be the result computed by $f(\cdot)$ on the itemset I'. This means that $m_{I'} = support(I')$, as is the case for FIM. To evaluate $minPI$, $F(\cdot)$ is used: $F(m_{I'}, m_1, ..., m_q) = \min_{i \in I'}\{m_{I'}/m_i\}$.

GLIMIT is used with the above instantiations of its framework to mine interesting complex co-locations, as shown in Figure 5.2. For comparison, an Apriori [11] style implementation will be used in the experiments.

The Apriori [11] and Apriori-like algorithms are *bottom up item enumeration* type itemset mining algorithms. Apriori works in a breadth first fashion, making one pass over the data set for each level expanded. This is in contrast to GLIMIT, which makes only one pass over the entire data set. In Apriori, a *candidate generation* step generates candidate itemsets (itemsets that may be interesting) for the next level, followed by a data set pass (*support counting*) where each candidate itemset is either confirmed as interesting, or discarded. The support counting step is computationally intensive as subsets of the transactions need to be generated. This is particularly problematic when the transaction width is large, as is the case for spatial co-location data that includes complex relationships. GLIMIT operates on completely different principles and does not have these drawbacks.

It is also worth noting that since all single itemsets are always interesting (by definition, their $minPI$ has the maximum value of 1), they cannot be discarded from the search. Note that were an FP-Growth style algorithm developed for this mining task, it would need to build an FP-Tree for the entire data set without any pruning. Hence, it is not a practical choice for this problem.

5.6 Mapping the Problem to GIM

GIM is more abstract than GLIMIT (which focuses only on itemset mining) and operates on a different (but related) framework and algorithm. Furthermore, while GLIMIT performs subset checking and requires that the entire PrefixTree remain in memory, both of these can be avoided in GIM; saving space and time. This was briefly discussed in section 3.11.

While the experiments in this chapter were performed using GLIMIT, it is worth showing how the problem can be solved directly in GIM:

- Each complex type is a *variable*, and complex maximal clique is a *sample*.
- Interaction vectors $x_{V'}$ contain the set of complex maximal clique IDs that contain V', where V' is a complex spatial co-location pattern. Suppose $x_{V'}$ is implemented as a bit vector.
- $a(x_{V'}, x_v) = x_{V'}\, AND\, x_v$, the bit-wise AND operation.
- $m_I(x_{V'}) = |x_{V'}|$, the number of set bits. This is the support of the interaction V'
- $M_I(\cdot)$ evaluates $minPI$ of V' by using the result of $m_I(x_{V'})$ and looking up the $m_I(x_v) : v \in V'$ using the sequence map. As explained in section 3.11, `store(·)` only needs to store $PrefixNode$s corresponding to single variables. Hence, the prefix tree is not stored in memory.
- $S_I(\cdot) = I_I(\cdot)$ and returns true iff the value computed by $M_I(\cdot)$ is at least equal to the $minPI$ threshold.

Recall that mining maximal cliques is performed using a specialist algorithm [12]. This step can also be performed using GIM, as described in Section 3.8.2.

5.7 Experiments

To evaluate the process presented in this Chapter, a real life two dimensional astronomy data set from the the Sloan Sky Digital Survey (SDSS) [1] was used. All galaxies from this data set were extracted, giving a total of $365,425$ objects. There were 12 *types* of galaxies. The distance threshold used for generating the maximal cliques was 1 Mega-parsec[1].

[1] The mega-parsec is an astronomical distance measure. See http://csep10.phys.utk.edu/astr162/lect/distances/distscales.html for details.

A total of 121,506 maximal cliques (transactions) were extracted in 39.6 seconds. These were processed in a number of ways (refer to Table 5.1 for examples) as described in Section 5.4:

- **Non-Complex**: All duplicate items (object types) were removed in the maximal cliques.
- **Complex w/o Negative**: *Positive* types were included: if an object type A occurred more than once in a maximal clique, it was replaced with A and $A+$. No negative types were included.
- **Complex w Negative**: The same as **Complex w/o Negative**, but *negative* types were included.

The following table describes the resulting sets of maximal cliques used for mining interesting patterns:

Maximal Clique Set	Items	Average Size (Transaction Width)
Non-Complex	12	1.87
Complex w/o Negative	21	2.69
Complex w Negative	33	13.69

Note that the the "Complex w Negative" data set is very large. It has 121,506 transactions (like the others), but each transaction has an average size of 13.7.

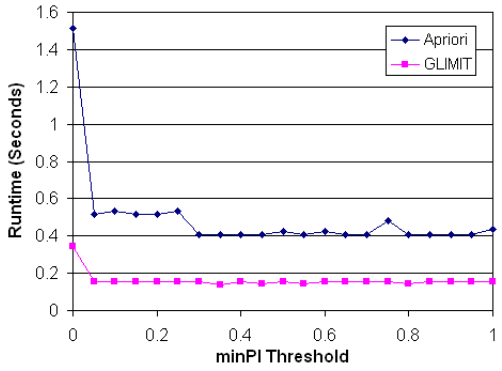
Since most co-location mining algorithms are based on the Apriori algorithm, this was used as the comparison. That is, both GLIMIT and Apriori were evaluated for the interesting pattern mining task of Figure 5.2.

Figure 5.5 shows the number of interesting patterns found on the different sets of cliques.

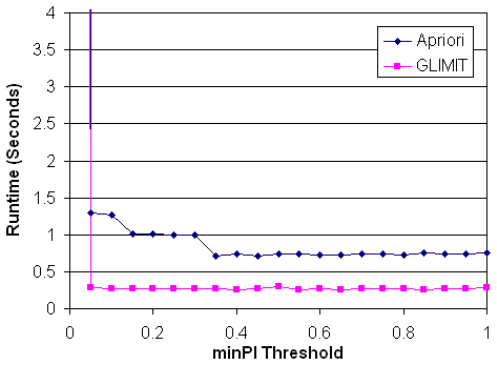
Figures 5.3(a), 5.3(b) and 5.3(c)[2] show the run time[3] of the pattern mining. It is clear that GLIMIT easily outperforms the Apriori technique. In particular, note the difference between the run-times when negative items are involved; namely, Figure 5.3(c). **For example, with a *minPI* threshold of 0.85, Apriori takes 33**

[2] An upper limit of 2,000 seconds (33 minutes) was set

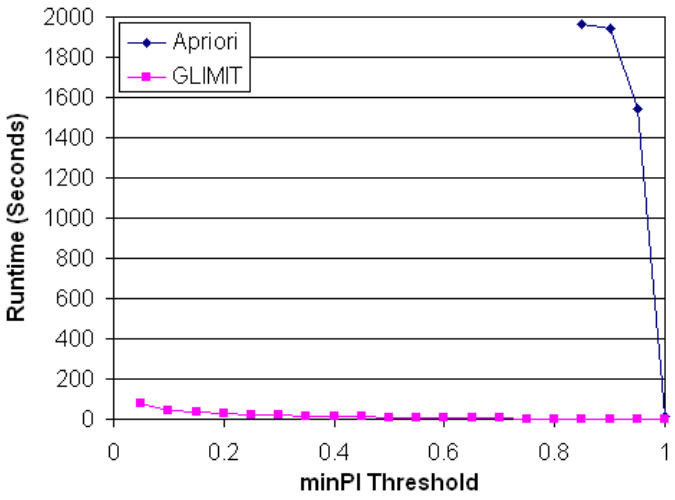
[3] Programs were implemented in Java and run on a laptop with a 2.0GHz Pentium 4M processor and Windows XP Pro.



(a) Runtime on non-complex maximal cliques.



(b) Runtime on complex maximal cliques without negative patterns.



(c) Runtime on complex maximal cliques with negative patterns.

Figure 5.3: Computational Performance. The *minPI* threshold was changed in increments of 0.05.

minutes **(1967 seconds), while GLIMIT takes only** 2 ***seconds*****. This is a difference of almost three orders of magnitude.**

As can be seen from the previous table, the use of negative types increases the average transaction width substantially. This has a large influence on the run time of the Apriori algorithm, due to the support counting step where all subsets (of a particular size) of a transaction must be generated. This is not true of GLIMIT, which runs in roughly linear time in the number of interesting patterns found, as can be seen in Figure 5.4. The "non-complex" and "complex w/o negative" data sets, due to their small average transaction width, may be considered very easy. The "complex w negative" data set is difficult for Apriori, but very easy for GLIMIT. Indeed, even with a *minPI* threshold of 0.05 it takes only 76 seconds to mine 68,633 patterns

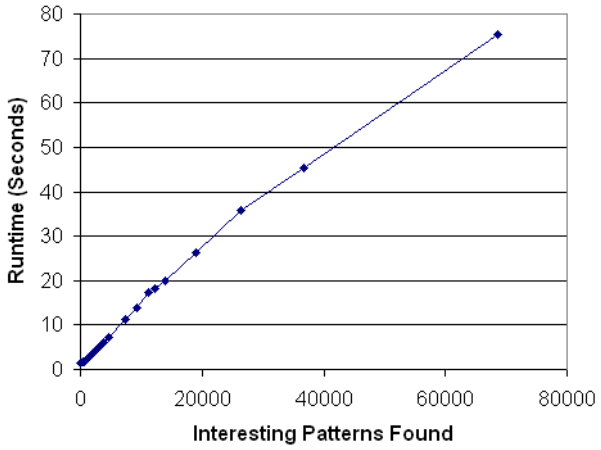


Figure 5.4: The run time of GLIMIT on complex maximal cliques with negative patterns, versus the number of interesting patterns found.

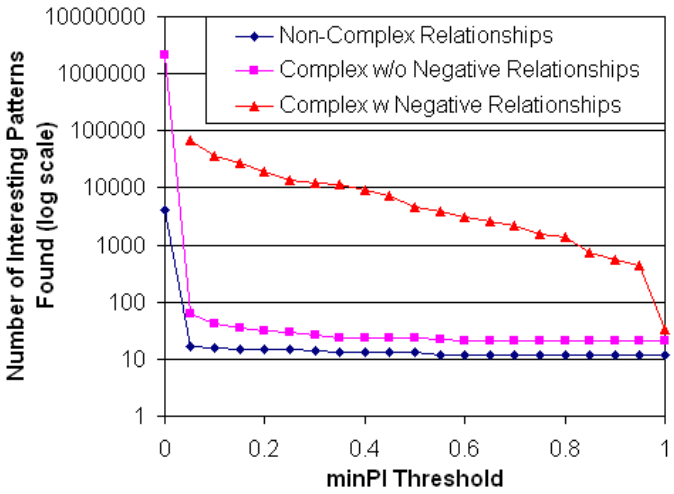


Figure 5.5: Number of interesting patterns found.

using GLIMIT.

5.8 Related Work

The expression "spatial data" was defined as location-based data by Judd [50]. However, a simple definition of a spatial database is a collection of data that contains information on an observable fact of interest, such as forest condition or pollution, and the location of an observable fact on the Earth. Spatial data consists of two types of attributes; the normal attributes, which are defined as non-spatial attributes, and spatial attributes that describe an instances location.

Huang et al. [49] define the co-location pattern as the presence of a spatial feature in the neighborhood of instances of other spatial features. They develop an algorithm for mining valid rules in spatial databases using an Apriori based approach. Their algorithm does not separate the co-location mining and interesting pattern mining steps like the KDD process in this Chapter. Also, they do not consider complex relationships or patterns. Specifically, their method cannot mine give complex rules such as $A \rightarrow B+$ or $B \rightarrow -C$ and they do not allow cliques to be connected to each other, which can lead to some cliques being ignored.

Monroe et al. [64] use cliques as a co-location patterns. Similar to the approach in this chapter, they separated the clique mining from the pattern mining stages. However, they do not use maximal cliques. They treat each clique as a transaction and use an Apriori based technique for mining association rules. Since they used cliques (rather than maximal cliques) as transactions, the counting of pattern instances is very different. They consider complex relationships within the pattern mining stage. However, their definition of negative patterns is different – they use infrequent types while the work in this Chapter is based on the concept of absence in *maximal cliques*. Therefore, in [64] a negative pattern does not necessarily mean that type is not present. Monroe et al. also used a different measure; $maxPI$. Furthermore, they define the positive relationship as a set of features that co-locates in a ratio greater than predefined threshold. Perhaps a method based on maximal cliques, as introduced in this Chapter, is simpler, leads to more useful semantics and avoids the problems caused by the fact that large cliques have many sub-cliques.

Arunasalam et al. [16] use a similar approach to [64]. They propose an algorithm called NP_maxPI which also uses the $maxPI$ measure. The proposed algorithm prunes the candidate itemsets using the *weak anti-monotonic* property of $maxPI$. They also use an Apriori based technique to mine complex patterns. A primary goal of their work is to mine patterns which have low support and high confidence. As with the work of [64], they did not use maximal cliques.

Zhang et al. [116] enhanced the algorithm proposed in [49] and used it to mine special types of co-location relationships in addition to cliques, namely; the *spatial star*, and *generic* patterns. Most related work makes use of anti-monotonic or weakly anti-monotonic measures. Morimoto [62], however, used a measure that is not anti-monotonic to mine a co-location pattern called the k-neighboring class set.

To the best of the authors knowledge, all previous work has used Apriori type algorithms for mining interesting co-location patterns. This work uses GLIMIT as the underlying pattern mining algorithm as already discussed in Section 5.5. Furthermore, this is the first work to apply GLIMIT on spatial data and with a measure

other than support.

5.9 Conclusion

This Chapter introduced the idea of using maximal cliques for complex pattern mining, which is fundamental to the approaches presented in this work. It was argued that complex patterns only make sense in the context of maximal cliques. Using maximal cliques also allowed the clique generation step to be split from the interesting pattern mining tasks and avoided the problem of redundant cliques. This Chapter presented a complete KDD process for the problem of mining complex spatial co-location patterns. This Chapter showed that the complex spatial co-location pattern mining problem can be mapped to the GLIMIT algorithm, and that this is a far more efficient solution than using the traditional Apriori style of algorithm, especially when complex patterns are involved. Previous work in co-location mining used Apriori style algorithms.

Since the problem in this chapter was one of the many influences in developing the generalised interaction mining (GIM) approach of Chapter 3, the problem can also be solved directly using GIM. Furthermore, recall that Chapter 3 showed how $maxPI$ can be applied to this problem efficiently using GIM (see section 3.12.1).

Chapter 6

Generalised Rule Mining

Rules are an important interaction pattern in data mining, but existing approaches are limited to conjunctions of binary literals, fixed measures and counting based algorithms. Rules can be much more diverse, useful and interesting! This work introduces and solves the *Generalised Rule Mining* (GRM) problem, which removes restrictions on the semantics of rules and redefines rule mining by functions on vectors. This abstraction is motivated through the introduction of three diverse and novel methods addressing problems including correlation based classification, finding interactions for improving regression models and finding probabilistic association rules in uncertain databases. Two of these methods are introduced in this chapter, while one is introduced in chapter 7. Furthermore, this approach can be applied to other methods, such in chapter 8.

The proposed GRM framework and algorithm allow methods not possible with existing algorithms, speed up existing methods, separate rule semantics from algorithmic considerations and lend an interesting geometric interpretation to the rule mining problem. The GRM algorithm scales linearly in the number of rules found and provides orders of magnitude speed up over fast candidate generation type approaches when these are applicable.

6.1 Introduction

Rules are an important pattern in data mining due to their ease of interpretation and usefulness for prediction. They have been heavily explored as association patterns [11, 22, 81, 47, 84], "correlation" rules [22, 108] and for associative classification [61, 60, 100]. These approaches consider only conjunctions of binary valued variables[1], use fixed measures of interestingness and counting based algorithms[2]. The rule mining problem can be generalised by relaxing the restrictions on the semantics of the antecedent as well as the variable types, and supporting any measure on rules. A *generalised rule* $A' \rightarrow c$ describes a relationship between a set of variables in the antecedent $A' \subseteq A$ and a variable in the consequent $c \in C$, where A is the set of possible antecedent variables and C is the set of possible consequent variables[3]. The goal in *Generalised Rule Mining* (GRM) is to find useful rules $A' \rightarrow c : A' \subseteq A \wedge c \in C \wedge c \notin A'$ given functions defining the measures and semantics of the variables and rules. Unlike in existing methods, variables do not need to be binary valued. Unlike in existing methods, semantics are not limited to conjunction.

This work introduces and solves the Generalised Rule Mining problem by proposing a vectorized framework and algorithm that are applicable to general-to-specific methods[4]. The framework is composed of five functions;

1. Rules are evaluated using a vector valued distance function $m_R(x_{A'}, x_c)$ applied to the vectors corresponding to the antecedent $(x_{A'})$ and the consequent (x_c) of the rule $A' \rightarrow c$.
2. An aggregation function $a_R(\cdot)$ incrementally builds $x_{A'}$ and implicitly defines the semantics of the rule.
3. $M_R(\cdot)$ allows complex evaluations requiring comparisons to less specific rules,
4. $I_R(\cdot)$ defines the interestingness of rules and search expansion criteria and
5. $I_A(x_{A'})$ allows (pre-emptive) antecedent pruning when possible.

Rule mining is a challenging problem due to its exponential search space in $A \cup C$. At best, an algorithm's run time is linear in the number of interesting rules it finds,

[1] The antecedent and consequent consist of a conjunction of literals that are either true or false.
[2] Such algorithms explicitly count instances/transactions that apply to a rule, typically through explicit counting, subset operations or tree/trie/graph traversals.
[3] Note that A and C do not need to be mutually exclusive.
[4] That is, methods where a less specific rule $A" \rightarrow c : A" \subset A'$ is mined before the more specific one $A' \rightarrow c$.

and the GRM algorithm is provably optimal in this sense. It also scales linearly in the dimensionality of the vectors, and can use space linear in the size of the database. The GRM algorithm in itself is very fast. It completely avoids "candidate generation" and does not build a compressed version of the data set – thus setting it apart from Apriori and FP-Growth. Instead it operates directly on vectors. Furthermore, the vectorization inherent in the framework's functions provides additional avenues for reducing the run time: On single processor architectures, vectorization allows automatic parallelisation and exploitation of machine level operations for bit-vectors, and optimizations for operations on floating point arrays (real vectors). On multiprocessor architectures, vectorization also provides a point for concurrentisation [105] while on supercomputer architectures, single instruction vector processing is directly supported [105].

By abstracting rule mining, the GRM framework separates the semantics and measures of rules from the algorithm used to mine them. The GRM algorithm can be exploited for any methodology map-able to the frameworks functions, such as [61, 60, 98, 103], especially generalized associative type patterns and mining classification rules. For example, methods based on counting such as support, confidence, lift, interest factor, all-confidence, correlation, significance tests and entropy. In particular, complete contingency tables can be calculated, including columns for subrules as required by complex, statistically significant rule mining methods [98, 103]. More interestingly though, it supports novel approaches including those with semantics unlike any existing method.

6.1.1 Contributions

The contributions of this work are as follows:

- It defines the *Generalized Rule Mining* (GRM) problem and proposes a vectorised framework that solves GRM using only functions on vectors. As a side effect, this provides a natural geometric interpretation of rule mining, which is very different to the counting interpretation in previous work. Together with the algorithm, this solves the generalized rule mining problem for general-to-specific rule mining with one variable in the consequent.
- It introduces the *vectorized* GRM algorithm, which efficiently solves any rule mining problem expressible in the GRM framework. It is *not* based on Apriori or FP-Growth or any other counting based algorithm. It also supports/exploits any mutual exclusion constraints on variables.

- To motivate and demonstrate GRM, two novel rule mining approaches are introduced:
  - First, *Probabilistic Association Rule Mining* (PARM) tackles association analysis in uncertain or probabilistic transaction databases. The required probability computations naturally fit into the vectorised GRM framework.
  - Secondly, *Conjunctive Correlation Rules* (CCRules) are used for an associative classifier. It uses the proposed *Correlation Improvement* technique to direct the search, which also has an interesting geometric interpretation.

  Aside: In addition to the motivational methods above, another technique called *Correlated Multiplication Rules* (CMRules) is developed in chapter 7. It finds multiplicative interactions and a method is presented for mining the best interaction terms for inclusion in linear (especially regression) models. This enables linear models to achieve non-linear decision boundaries by using the antecedents of CMRules as composite features and is the first rule mining approach with multiplication semantics.

6.1.2 Organisation

The remainder of this chapter is organised as follows: Section 6.2 places the this work in context of related work. Section 6.3 presents two novel techniques that are solved efficiently using GRM. Section 6.4 presents the GRM framework. Section 6.5 describes the GRM algorithm. Section 6.6 presents experimental results and the chapter is concluded in section 6.7.

6.2 Related Work

Most existing rule mining methods are used for associative pattern mining or classification. These only consider rules with conjunctive semantics of binary literals and use counting approaches in their algorithms. Other than border traversal based techniques for maximal or closed item-sets, they use general-to-specific searches. Association rule mining methods [11, 47, 81] typically mine item-sets before mining rules. Unlike GRM, they do not mine rules directly. Itemset mining methods are often extended to rule based classification [110, 61, 100]. The algorithms can be categorized into Apriori-like approaches [11] characterized by a breadth first search through the

item lattice and multiple database scans, tree based approaches [47] characterized by a traversal over a pre-built compressed representation of the database, projection based approaches [100] characterised by depth first projection based searches and vertical approaches [81, 34, 96] that operate on columns. Vertical bit-map approaches [81, 96] have received considerable interest due to their ability to outperform horizontal based techniques. Of existing work, the vectorized approach in GRM is most similar to the vertical approach. However, GRM is not limited to bitmaps or support based techniques; for example, unlike any previous work it can usefully and meaningfully handle real vectors as demonstrated by PARM and CMRules. It also solves a different problem, namely, the generalised rule mining problem, and mines rules directly – without first mining sets. It also runs in provably linear time in the number of interesting rules output.

Rule based classification is a major application area for rules with one variable in the consequent [110, 60, 61, 100]. Approaches in literature are specific to one measure or approach, do not generalize well and are based on the above association / item set mining algorithms. Rules based on decision trees [76] or rule induction [27] have different mining approaches generally not compatible with those considered here.

The "generalisation" of rules in this paper applies to the ability to support many different semantics, variable types and interestingness measures. This is different to the "generalization" of association rules in the literature, where it refers to quantitative rules [84, 78], correlations [22] or hierarchical rules. Quantitative rules [84] consider the number of items bought in a transaction and mine rules with quantity ranges. More recently, the term has referred to relationships between weighted sums of variables [78], though this is an optimisation problem rather than a rule mining problem. Within the GRM framework, such databases correspond to integer valued variable vectors. However, the rules are still conjunctions of binary valued literals. Correlation rules [22] are "general" in that they use a different measure on rules; thus "generalizing" association rules from support and confidence to correlation. But like other approaches, this just uses another, fixed, measure. Since GRM is a true framework, unlike existing approaches it avoids limiting the rule definition and solves the problem at the abstract level. As far as the author is aware, no existing rule mining approach considers real valued vectors, expands the rule definition to non-conjunctive semantics, allows a wide range of measures, or attempts to solve the problem at this abstracted level.

The mutually exclusive constraints considered in this paper are not hierarchical [85] and are primarily used for classification using conjunctive rules where values have been discretised. No work was found that considers rule mining geometrically. Re-

lated work pertaining to the motivational methods introduced in this chapter (that is, PARM and CCRules) is covered in the corresponding sections.

6.3 Novel and Motivational Methods Solved Using GRM

This section presents two very different and novel techniques that are solved efficiently using GRM. These problems can be solved orders of magnitude faster with GRM than using a suitable alternative method. Furthermore, chapter 7 will introduce another novel technique that can only be solved with GRM. In addition to these novel methods, section 6.4 will show how existing techniques such as support based rules are solved using the GRM framework.

6.3.1 Probabilistic Association Rule Mining (PARM)

In a probabilistic database D, each row r_j contains a set of observations about variables $A \cup C$ together with their probabilities of being observed in r_j. Probabilistic databases arise whenever there is uncertainty or noise in the data. For example, in the medical domain each row may correspond to a patient, the variables are medical conditions and the probabilities capture the likelihood that the patient has (or will get) the condition based on risk factors or tests. For instance, prenatal tests to determine chromosomal or genetic disorders in the fetus, such as cystic fibrosis, return probabilities. Risk factors such as smoking, sex, family history, etc can also provide probability estimates of diseases. In such databases, *Probabilistic Association Rules* can show interesting patterns while taking into account the uncertainty of the data. Traditional association analysis cannot deal with probabilistic databases. Previous work such as [25, 26, 58, 7, 57] has examined expected frequent itemsets, that is, the itemset mining task where itemsets with an *expected support above minSup* are mined. These do not consider rules. Furthermore, previous work has used Apriori [26, 25] or FP-Growth style approaches [58, 7, 57]. No previous work that the author is aware of has cast probabilistic pattern mining in terms of vectors.

Problem Definition: *Probabilistic Association Rule Mining* (PARM): find probabilistic association rules $A' \rightarrow c$ where the expected support $E(s(A' \rightarrow c)) = \frac{1}{n}\sum_{j=1}^{n} P(A' \rightarrow c \subseteq r_j)$ and expected confidence $exp\_conf(A' \rightarrow c)$ (defined later) are above thresholds $minExpSup$ and $minExpConf$ respectively. Under the assumption that the variables' existential probabilities in the rows are determined under independent observations, $P(A' \rightarrow c \subseteq r_j) = \Pi_{a \in A'} P(a \in r_j) \cdot P(c \in r_j)$.

The PARM problem could be solved using an Apriori style algorithm adapted for rules (this is not straightforward) and where subset checking is replaced by probability evaluation. However, this leads either to large space requirements or repeated work in the probability calculations (consider how $P(A' \rightarrow c \subseteq r_j)$ is calculated when one adds a variable to the antecedent). It also has the usual run time disadvantages of Apriori.

In the *GRM* model however, each variable is represented by a probability vector x_i expressing the probabilities $x_i[j] = P(i \in r_j) : j \in \{1, n\}$. That is, the probabilities that the variable i exists in row j of the database. As will be further explained in section 6.4, *all* the $\{P(A'' \rightarrow c \subseteq r_j) : r_j \in D : A'' \subseteq A'\}$ can be calculated easily and efficiently by incremental element-wise multiplication of individual vectors using an appropriate $a_R(\cdot)$ function. The GRM algorithm's use of $a_R(\cdot)$ ensures that there is no duplication of calculations throughout the mining process while keeping space usage to a minimum through its depth first approach.

By the definition of $P(A' \rightarrow c \subseteq r_j)$, adding variables to A' increases the number of probabilities multiplied together. Hence, it can easily be shown that the following lemma holds.

Lemma 6.1. *expected support is downwards closed (anti-monotonic):* $E(s(A' \rightarrow c)) \leq E(s(A'' \rightarrow c)) : A'' \subseteq A'$

To complete the PARM method, define the *expected confidence* of a rule $A' \rightarrow c$ as $exp\_conf(A' \rightarrow c) = E(s(A' \rightarrow c))/E(s(A'))$ where $E(s(A')) = \frac{1}{n}\sum_{j=1}^{n} P(A' \subseteq r_j)$ and filter out all rules not meeting the $minExpConf$ threshold. The expected confidence measures the degree of association between A' and c[5]. Note that the expected support and expected confidence reduce to the usual definitions of support and confidence [88] when the database has no uncertainty.

6.3.2 Conjunctive Correlation Rules for Classification (CCRules)

This section presents a rule mining method that finds conjunctive rules where the antecedent is highly correlated with the consequent, and uses these rules in a classification method. These rules, together with the method by which they are mined – called *Correlation Improvement* – also have an interesting geometric interpretation

[5]Note that defining the expected confidence as the expectation (over all rows r_j) of the *probabilistic confidences* $P(A' \rightarrow c \subseteq r_j)/P(A' \subseteq r_j)$ is pointless under the independence assumption, as $\frac{P(A' \rightarrow c \subseteq r_j)}{P(A' \subseteq r_j)} = P(c \subseteq r_j)$.

and therefore illustrate this aspect of the GRM framework. In particular, the rules are mined in such a way that a vector representing the antecedent of the rule moves 'closer' to the vector corresponding to the consequent in comparison to more general rules. Furthermore, the ability of the GRM algorithm to exploit mutual exclusion amongst variables is also of benefit for these rules.

Conjunctive rules using correlation measures have been studied in the literature, though all are quite different to those presented in this paper; [22] uses a χ^2 test to measure the significance of a correlation, but measures correlation by independence – *not* by Pearson's correlation. [108] uses Pearson's correlation, but this is applied to item pairs, not rules. FOSSIL [40] mines rules for classification using a heuristic based only on Pearson's correlation, but it is an inductive logic programming approach. When applied to binary data, Pearson's correlation reduces to the ϕ-coefficient. While the ϕ-coefficient is often used to evaluate rules mined by other methods [88], the author is not aware of any purely correlation based approach such as *Correlation Improvement*.

In the proposed CCRules method, A is a set of attribute-value pairs as would be the case when one has binary features, nominal attributes or discretised numeric attributes. C is the set of possible classes. The antecedent of each rule is a *conjunction* of attribute-value pairs. For example, suppose we have the "Adult" / "Census Income" Data set[6] available from the UCI Machine learning repository [2]. In this data set, the task is to predict whether a persons income is above $50,000\,USD$ based on census data. A rule in this domain might look like:

$$30 \leq age < 40 \wedge education = Doctorate \wedge sex = female \rightarrow income > 50K$$

If the rule is a 'good' rule and the antecedent holds, then the rule – in conjunction with other matching rules – may be applied to classify a new instance. A 'good' rule in this work is a rule where the antecedent is correlated with the consequent, and more so than all less specific rules.

Pearson's correlation coefficient between two variables v and c may be written as

$$r_{v,c} = \frac{\sum_{i=1}^{n}(x_v[i] - \bar{x_v})(x_c[i] - \bar{x_c})}{\sqrt{\sum_{i=1}^{n}(x_v[i] - \bar{x_v})^2}\sqrt{\sum_{i=1}^{n}(x_c[i] - \bar{x_c})^2}}$$

where $r_{v,c} \in [-1, 1]$, $\bar{x_v}$ is the mean of v and $x_v[i]$ is the ith sample of variable v. In order to use this to evaluate a conjunctive rule with binary variables, consider a

[6] http://archive.ics.uci.edu/ml/datasets/Adult

$A' \rightarrow c$	c	$\neg c$	$n_{i+} = \sum_j n_{ij}$
A'	n_{11}	n_{10}	n_{1+}
$\neg A'$	n_{01}	n_{00}	n_{0+}
$n_{+j} = \sum_i n_{ij}$	n_{+1}	n_{+0}	$n = \sum_{i,j} n_{ij}$

Figure 6.1: Contingency table for a rule $A' \rightarrow c$.

vector $x_{A'}$ as containing a 1 for those samples (instances) that match the antecedent, and 0 otherwise. Similarly, the values $x_c[i]$ is 1 if the ith instance has class c and 0 otherwise. When applied to such binary valued data, it can be shown that Pearson's correlation coefficient reduces to the $\phi - coefficient$:

$$C(A' \rightarrow c) = \frac{n \cdot n_{11} - n_{1+} \cdot n_{+1}}{\sqrt{n_{1+} \cdot (n - n_{1+}) \cdot n_{+1} \cdot (n - n_{+1})}}$$

where n_{11} is the total number of instances matching $A' \rightarrow c$ and the other ns are defined in the contingency table of Table 6.1.

6.3.3 Directing the Search by Correlation Improvement

Recall that the goal is to find highly correlated rules. The simplest approach is to attempt to find rules with a correlation above some user defined threshold. However, it is problematic to direct the search space by only expanding rules with correlation above a threshold for two reasons.

- First, it introduces an arbitrary parameter to which the approach becomes sensitive.
- More subtly, since correlation is not downwards closed, it also introduces a dependency on the order in which variables are added to the antecedent. This could be addressed by "forcing" anti-monotonicity as a heuristic but the limitation inherent in absolute threshold based techniques remains.

Instead, the following approach is used: A variable should only be added to the antecedent of a rule if it *improves* the rule compared to its generalizations. That is, if the variable increases the correlation compared to those less specific rules having fewer variables in the antecedent. The *Correlation Improvement* (CI) measures this improvement;

Definition 6.2. The *Correlation Improvement* is $CI(A' \rightarrow c) = C(A' \rightarrow c) - \max_{a \in A'}\{C(A' - \{a\} \rightarrow c)\}$ where $A' - \{a\} \rightarrow c$ is a less specific *sub rule* obtained by removing variable a from the antecedent.

Note that $A' - \{a\} \rightarrow c$ is a generalization (a less specific rule) that therefore applies to more instances, while $A' \rightarrow c$ is more specific rule that applies to less instances. For an empty antecedent (the base case), $CI(\emptyset \rightarrow c) = C(\emptyset \rightarrow c)$. The *Correlation Improvement* is positive if the rule to which it is applied has a higher correlation than any of its immediate generalizations. This means it is a better predictor of the consequent variable than any of the less specific rules.

Therefore, the Correlation Improvement approach will find rules where the antecedent is correlated with the class it predicts, and the search builds more specific rules only if they improve on the existing rule base. The property that a more specific rule will only ever be mined if it is better than all sub rules is very important when such rules are applied to classification or used for prediction. Of all rules matching an instance, the most specific one should be the best. This method also avoids contradictions when multiple rules are used to classify an unseen instance. Another important consideration is that in a good rule $A' \rightarrow c$, the antecedent A' should be more correlated with what it predicts – that is, c – than with the alternative(s) $c' \in C : c \neq c'$. It turns out that this must always be the case in binary data, as is shown and discussed in section 6.8.

Problem definition: *Correlated Classification Rules* (CCRules): Find all CCRules with $CI(A' \rightarrow c) > minCI$, where $minC \geq 0$ is a user defined threshold. (Recall that A' is interpreted as a conjunction of attribute-values$\wedge_{i \in A'} a_i$).

Note that the base case ensures that all rules are positively correlated, and that $\emptyset \rightarrow c$ will always be expanded.

Since the attribute-value pairs are binary valued, this approach can be implemented in the GRM framework using binary vectors and bit-wise operations. This enables the exploitation of machine level operations. Section 6.4 explains this in more detail.

6.3.3.1 CCRules for Classification

CCRules are used for classification as follows:

1. CCRules are mined using the GRM algorithm. Then each rule is assigned a

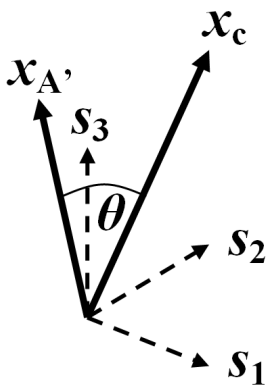


Figure 6.2: The rule $A' \to c$ viewed geometrically: The antecedent and consequent of $A' \to c$ in the space spanned by the first three samples in the database.

score reflecting how useful it is expected to be when classifying new instances:

$$Score(A' \to c) = C(A' \to c) \cdot CI(A' \to c)$$

That is, the *correlation* multiplied by the *correlation improvement*. This is done because a highly correlated rule is desirable, but only if it improves on its less specific sub-rules.

2. In order to classify an unseen instance, the mean score is calculated over all matching rules predicting a class. The instance is classified according to the class with the highest mean score. This ensures that each matching rule contributes to the classification while classifying using rules with high scores. Recall that there cannot be a contradiction between specific rules and less specific ones due to the Correlation Improvement method.

Experiments show that this approach performs well.

6.4 Generalised Rule Mining (GRM) Framework

This section presents the vectorised GRM framework, shows how the motivational methods fit into it and describes the geometric interpretation. Recall that elements of $A \cup C$ are called *variables* and the goal is to find useful rules $A' \to c : A' \subseteq A \wedge c \in C \wedge c \notin A'$, where the antecedent A' can have any semantics. For example, variables could be binary valued as in CCRules or real valued as in PARM and in CMRules (which will be introduced in chapter 7). CMRules has multiplicative semantics, while CCRules and PARM have conjunctive semantics. Also recall that in

the GRM framework, each possible antecedent $A' \subseteq A$ and each possible consequent $c \in C$ are expressed as vectors, denoted by $x_{A'}$ and x_c respectively. As indicated in figure 6.2, these vectors exist in the space X, the dimensions of which are *samples* $\{s_1, s_2, ..., s_n\}$ – depending on the application these may be instances, transactions, rows, etc. The database is the set of vectors corresponding to individual variables, $D = \{x_v : v \in A \cup C\}$. The space X is dependent on the type of variables considered. This work presents techniques with variables in $\mathbb{R}^n$ and in $\{0,1\}^n$.

Good rules have high prediction power. Geometrically, in such rules the antecedent vector is "close" to the consequent vector.

Definition 6.3. $m_R : X^2 \to \mathbb{R}^k$ is a set of k distance measures between the antecedent and consequent vectors $x_{A'}$ and x_c. $m_R(x_{A'}, x_c)$ evaluates the quality of the rule $A' \to c$. k is fixed.

That is, it is some form of distance metric (or metrics) that evaluate how useful the rule is expected to be.

In *PARM* (section 6.3.1), $m_R(\cdot)$ is the expectation function and calculates the expected support: $m_R(A' \to c) = \frac{1}{n} \sum_{j=1}^{n} x_{A'}[j] * x_c[j]$. Geometrically, this is the scaled dot product of $x_{A'}$ and x_c: $m_R(A' \to c) = \frac{|x_{A'}||x_c|}{n} x_{A'} \cdot x_c$. CCRules (section 6.3.2) uses Pearson's correlation coefficient. Geometrically, this is the cosine of the angle θ between $x_{A'}$ and x_c (see figure 6.2). In CCRules the attribute-value pairs are binary valued variables. It this case, recall that $C(A' \to c) = \frac{n \cdot n_{11} - n_{1+} \cdot n_{+1}}{\sqrt{n_{1+} \cdot (n - n_{1+}) \cdot n_{+1} \cdot (n - n_{+1})}}$ (the ϕ-coefficient), where n_{11} is the number of instances matching $A' \to c$ and the other ns are defined in the contingency table of figure 6.1. This is advantageous since these are counts (a.k.a frequencies). Any method based on counting can be implemented using bit-vectors in the GRM framework (sparse methods outlined in section 3.15 can of course also be applied). Each variable corresponds to a binary literal that is true or false in the samples (instances, records, etc). A bit is set in $x_{A'}$ (x_c) if the corresponding sample contains A' (c). Then, the number of samples containing A', $A' \to c$ and c are simply the number of set bits in $x_{A'}$, $x_{A'}\, AND\, x_c$ and x_c respectively. From these counts (n_{1+}, n_{11} and n_{+1} respectively) and the length of the vector, n, a complete contingency table can be constructed as in figure 6.1. Using this, m_R can evaluate a wide range of measures such as confidence, interest factor, lift, ϕ-coefficient and even statistical significance tests. For example, all association rules with a single variable in the consequent can be mined and evaluated with any of these measures. Geometrically, in counting based applications m_R is the dot-product; $m_R(A' \to c) = x_{A'} \cdot x_c = n_{11}$.

Since x_c corresponds to a single variable it is readily available as $x_c \in D$. This is also the case for all $x_a : a \in A$. However, the $x_{A'} : A' \subset A \wedge |A'| > 1$ required for the evaluation of $m_R(\cdot)$ on rules with $|A'| > 1$ must be calculated. These are built incrementally from vectors $x_a \in D$ using the *aggregation function* $a_R(\cdot)$:

Definition 6.4. $a_R : X^2 \to X$ operates on vectors of the antecedent so that $x_{A' \cup a} = a_R(x_{A'}, x_a)$ where $A' \subseteq A$ and $a \in (A - A')$.

In other words, $a_R(\cdot)$ combines the vector $x_{A'}$ for an *existing* antecedent $A' \subseteq A$ with the vector x_a for a new antecedent element $a \in A - A'$. The resulting vector $x_{A' \cup a}$ represents the larger antecedent $A' \cup a$. In this way, the vector representing the antecedent can be built incrementally. This is equivalent to the $a_I(\cdot)$ function in the GIM framework of chapter 3. Note that this vector is the same as if it were calculated from the original data set, but rather than examining the original data set, it requires only one of the vectors (x_a) since the information from the rest is already represented in $x_{A'}$. This property can be exploited to allow the algorithm to efficiently evaluate the rules without recomputing vectors or scanning the data set to construct $x_{A' \cup a}$.

More importantly however, note that $a_R(\cdot)$ *also defines the semantics of the antecedent of the rule*. By defining how $x_{A' \cup a}$ is built, it must implicitly define the semantics between elements of $A' \cup a$. That is, what it means to add a variable to the antecedent of a rule.

For rules with a conjunction of binary valued variables such as CCRules and association rules, vectors are represented as bit-vectors and hence $a_R(x_{A'}, x_a) = x_{A'}\, AND\, x_a$ defines the required semantics; bits will be set in $x_{A' \cup a}$ corresponding to those samples that are matched by the conjunction $\wedge_{a_i \in A'} \wedge a$. In PARM (section 6.3.1), the vectors contain probabilities. Since the antecedent vector is defined by $x_{A'} = \Pi_{a \in A'} P(a \in r_j)$, $a_R(\cdot)$ is defined by element-wise multiplication: $a_R(x_{A'}, a_a)[j] = x_{A'}[j] * x_a[j]$. PARM is interpreted using conjunctive semantics.

While $m_R(\cdot)$ and $a_R(\cdot)$ suffice for many measures, it often occurs that a rule $A' \to c$ needs to be compared with its sub-rules $A" \to c : A" \subset A'$. This is particularly useful in order to find more specific rules that improve on their less specific sub-rules. Geometrically, this means the antecedent of a rule can be built by adding more variables in such a way that the corresponding vector $x_{A'}$ moves closer to the vector representing the consequent of the rule x_c. This is exactly what the *Correlation Improvement* technique does. Examples from the literature that require comparison to sub-rules include [103, 98]. The following function supports such behaviour.

Definition 6.5. $M_R : \mathbb{R}^{k \times |\mathcal{P}(A')|} \rightarrow \mathbb{R}^l$ is a measure that evaluates a rule $A' \rightarrow c$ based on the value computed by $m_R(\cdot)$ for any rule $A'' \rightarrow c : A'' \subseteq A'$. l is fixed.

$M_R(\cdot)$ does not take vectors as arguments – it evaluates a rule based on values that have already been calculated. This is important as it enables the algorithm to perform only one vector calculation per rule. Not that this is for algorithmic efficiency purposes only and does not limit the scope of the framework in any way. If $M_R(\cdot)$ does not need access to any sub-rules to perform its evaluation, it is called *trivial* since $m_R(\cdot)$ can perform the function instead. A *trivial* $M_R(\cdot)$ simply returns $m_R(\cdot)$ and has advantages in terms of space and time complexity (section 6.5).

In PARM, $M_R(\cdot)$ is trivial. The *Correlation Improvement* method is implemented using $M_R(\cdot)$ according to definition 6.2. Geometrically, since $C(A' \rightarrow c) = cos(\theta)$ and $CI(\cdot)$ must be positive, the search progresses by adding variables to the antecedent in a way that the antecedent vector moves closer to the consequent vector in terms of the subtended angle θ. In CCRules, variables will only be added if they improve the correlation with the class to be predicted. For counting based approaches, $M_R(\cdot)$ can be used to evaluate measures on more complex contingency tables such as those in [103, 98] and chapter 8. For example, to evaluate whether a rule significantly improves on its less specific sub-rules by using Fisher's Exact Test (see chapter 8). Together with I_R below, it can also be used to direct and prune the search space – even 'forcing' a measure implemented in m_R to be downward closed.

The final component of the framework defines what rules are *interesting*. Interesting rules are those that are

1. desirable and should therefore be output and
2. should be further improved in the sense that more specific rules should be mined by the GRM algorithm.

Definition 6.6. $I_R : \mathbb{R}^{k+l} \rightarrow \{true, false\}$ determines whether a rule $A' \rightarrow c$ is *interesting* based on the values produced by $m_R(\cdot)$ and $M_R(\cdot)$. Only interesting rules are further expanded and output.

In other words, more specific rules (i.e. with more variables in the antecedent) will only be considered if $I_R(\cdot)$ returns true. The simplest implementation of $I_R(\cdot)$ is to return true if $M_R(\cdot)$ is above (below) a threshold. For simplicity, both interestingness

concepts have been combined in $I_R(\cdot)$. Separating them, as is done in GIM with $I_I(\cdot)$ and $S_I(\cdot)$ (section 3.2) is of course also possible.

In PARM, the search space can be pruned by the expected support (lemma 6.1). Hence $I_R(A' \rightarrow c)$ returns *true* if and only if $m_R(A' \rightarrow c) \geq minExpSup$. For Correlation Improvement, the desired search strategy is achieved when I_R returns true for $A' \rightarrow c$ if and only if $CI(A' \rightarrow c) > minCI$.

Sometimes it is possible to determine that a rule is not interesting based purely on the antecedent. For example, in PARM the expected support of the antecedent is always less than that of the rule and so we can avoid unnecessary computation of rules. This pre-emptive pruning is defined by $I_A(\cdot)$:

Definition 6.7. $I_A : X \rightarrow \{true, false\}$. $I_A(x_A) = false$ implies $I_R(\cdot) = false$ for all $A' \rightarrow c : c \in C$.

The framework can accommodate any approach where a rule can (or must) be examined after its generalizations are examined. In other words, it accommodates bottom up approaches. Beyond that, the order in which rules are examined is up to the algorithm and complexity considerations.

6.5 Generalised Rule Mining Algorithm

The GRM algorithm efficiently solves any problem that can be expressed in the framework. It is optimal in the sense that it uses time linear in the number of rules found. It also uses space linear in the size of the data set. To understand the algorithm, it is necessary to understand the The Categorised Prefix Tree first, part of which involves the ability to exploit mutual exclusion constraints.

6.5.1 Mutual Exclusion Constraints

Often, groups of variables are mutually exclusive. For instance, when numeric attributes have been discretised, an attribute can take on only one of a set of values and each of these attribute-value pairs becomes a binary variable. The reader may recall the example for CCRules in section 6.3.2, where for example an attribute *age* is split into different ranges. Of course a person can only have an age in one range, and therefore the different ranges are mutually exclusive. It is pointless to check rules which contain the same attribute but with different values if these are mutually

exclusive, as no instances can exist with this property. Avoiding such unnecessary computation saves computational resources. A second source of mutual exclusion occurs when a user does not require certain combinations of variables to be examined as they are not interested them.

Such *intrinsic* and *extrinsic constraints* can be expressed through a *categorization* where variables in the same category are mutually exclusive. For example, all attribute-value pairs with the same attribute will correspond to one category. Variables that have no constraints are simply placed in categories by themselves. Exploiting such constraints reduces the search space from $O(2^{|A|} \cdot |C|)$ to $O(|C| \cdot \Pi_{i=1}^{m}(n_i+1))$, where n_i is the number of variables in the ith category. The GRM algorithm fully and implicitly exploits all constraints expressible by mutual exclusion through the use of a Categorised Prefix Tree.

6.5.2 Categorized Prefix Tree

The *Categorized Prefix Tree (CPT)* can efficiently store rules in a compressed format. The reader should keep in mind however, that *depending on the requirements of M_R, the Categorized Prefix Tree often does not need to be stored at all.*

The CPT is an important concept in the algorithm. The following rules define it: First, an arbitrary but fixed order is chosen on the variables – in this chapter, ascending order will be used. Variables in C *must* always be first in the order. Each node in the CPT (a *PrefixNode*) has a label corresponding to a variable $v \in A \cup C$. The root node is special, and is labeled with ∞. The CPT is constructed so that each node can only have a parent with a label greater than it's own label and not in its category.

Figure 6.3 shows a 'full' CPT in that it contains all possible rules given the set of variables and categories. In the figure, the variables $\{a, b\}$, $\{1, 2\}$ and $\{3, 4\}$ are mutually exclusive so the categorization is $\{\{a, b\}, \{1, 2\}, \{3, 4\}\}$. Each non-leaf node in a complete tree represents an antecedent $A' \in A$ and each leaf node (grey in the figure) represents a complete rule $A' \rightarrow c : c \in C$. Then rules can be reconstructed by traversal toward the root, which corresponds to the empty antecedent $A' = \emptyset$. When $M_R(\cdot)$ is non-trivial, the CPT can efficiently store rules in a compressed format through prefix sharing. Otherwise, only the current path the algorithm is processing is in memory. A *Complete Categorized Prefix Tree (CCPT)* such as shown in figure 6.3 is a 'full' CPT in that it contains all possible rules given the set of variables and categories. A *complete* CPT therefore also represents the *worst case* search space of the rule mining problem (when categories are exploited).

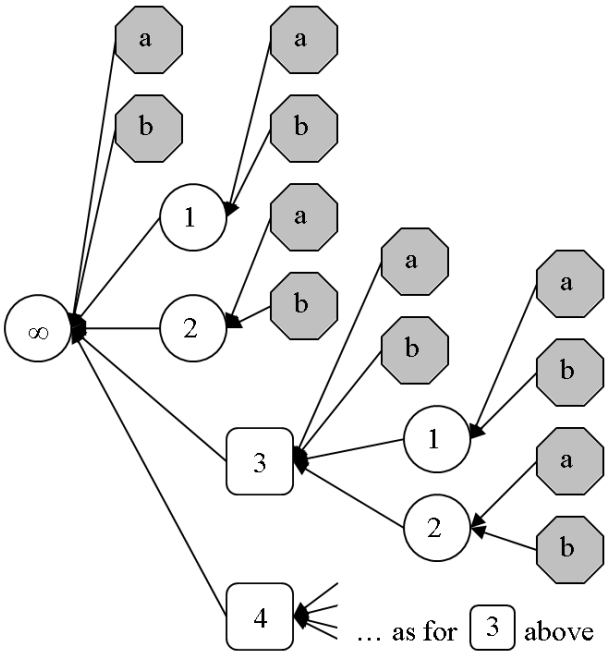


Figure 6.3: Example of a *Complete* (full) *Categorized Prefix Tree*. $A = \{1, 2, 3, 4\}$, $C = \{a, b\}$, and the categorisation is $\{\{a, b\}, \{1, 2\}, \{3, 4\}\}$.

6.5.3 Generalized Rule Mining Algorithm

The Generalized Rule Mining algorithm (algorithm 6.1) works by performing a strict depth first search (i.e. sibling nodes are not expanded until absolutely necessary), expanding nodes in increasing order and calculating vectors along the way. There is absolutely no "candidate-generation". The search is limited according to the interestingness function $I_R(\cdot)$ and $I_A(\cdot)$ and it progresses in depth by *joining sibling nodes* in the $PrefixTree$, thus auto-pruning. Vectors are calculated incrementally along a path in the search using $a_R(\cdot)$. This means that there are never any vector re-computations while at the same time maintaining optimal memory usage. Indeed, one expansion requires only one application of $a_R(\cdot)$ regardless how complex the rule. This is very important. The GRM algorithm *automatically* avoids considering rules that would violate the mutual exclusion constraints by carrying forward the categorization to the sibling lists ($joinTo$), and only joining siblings if they are from different categories. The search space can be *automatically* pruned (i.e. without requiring explicit checking, thus saving vector calculations) in two ways, according to the definition of $I_R(\cdot)$;

- First, if a rule $A' \cup a_1 \rightarrow c$ is not interesting, then rules $A' \cup a_2 \cup a_1 \rightarrow c$ do not have to be considered since they are more specific version of $A' \cup a_1 \rightarrow c$. For

example, in figure 6.3, if $1 \rightarrow a$ was not interesting, then $3,1 \rightarrow a$ would not need to be examined by the definition of $I_R(\cdot)$. This is automatically achieved by maintaining a list of siblings ($joinTo$), and only joining sibling nodes. Note that $A' \cup a_2 \rightarrow c$ and $A' \cup a_1 \rightarrow c$ are siblings in the CPT. Recall that only interesting rules as specified by $I_R(\cdot)$ are to be expanded, and therefore only interesting rules become siblings, achieving this pruning automatically.

- Secondly, if no rules with the antecedent A' are interesting, then that node is not further expanded. For example, if neither $3 \rightarrow a$ or $3 \rightarrow b$ are interesting in figure 6.3, then the complete sub-tree rooted at 3 can be pruned. This is called *prune early* functionality and implements the semantics of $I_R(\cdot)$.

In algorithm 6.1, evaluateAndSetM$_R(\cdot)$ evaluates M_R and sets $value_M$ of the *PrefixNode*. Recall that if M_R is *non-trivial*, its evaluation requires the $value_m$s of sub rules. In this case, store$(\cdot)$ stores the $PrefixNode$ in an index structure for later use by evaluateAndSetM$_R(\cdot)$. This means that the CPT will be built in memory as references to its leaf nodes is maintained. A suitable index structure would be a hash-table due to the constant look-up time that can be exploited by evaluateAndSetM$_R(\cdot)$. If M_R is trivial, store$(\cdot)$ does nothing and rules (and hence the entire *Categorized Prefix Tree*) *are not kept in memory*[7]. The outputRule$(\cdot)$ function provides rules (as $PrefixNode$s) to client code. For example, to output the rule to a file or to maintain the top k-rules.

Despite the search being depth first, the following holds, proving correctness.

Lemma 6.8. *All sub-rules $A'' \rightarrow c : A'' \subset A'$ are examined before $A' \rightarrow c$ is examined.*

Proof. The algorithm progresses through the search space by joining existing PrefixNode *siblings* together, creating antecedents or complete rules that are one variable larger than the two original sibling nodes. Suppose for the purpose of contradiction that a rule $r = A' \rightarrow c$ exists but a sub-rule of it is mined later. Proceed by showing that each sub-rule $A' - a \rightarrow c : a \in A'$ has already been mined, so that the result follows by induction. First, note that each rule can be represented by a *sequence* of PrefixNodes, which can be constructed in reverse by traversal from c towards the root. The immediate sub-rules of r can be obtained by removing one variable from the antecedent at a time. Suppose $a \in A'$ is removed, so that $r = S_p \cup a \cup S_s \rightarrow c$

[7] algorithm 6.1 assumes a garbage collector, so such rules – and hence the entire CPT except for the current search path – are garbage collected.

where S_p and S_s are the prefix and suffix (either potentially empty) of the antecedent (sequence) respectively. Since the expansion of the search is done in depth first fashion and with increasing order amongst the siblings (according to their variables), $S_p \cup S_s$ must be expanded first, since by definition the sequences in the *PrefixTree* appear in *decreasing* order. Since this is true for all $a \in A'$, the result follows by induction and contradiction. □

6.5.4 Complexity

Theorem 6.9. *The run time complexity is at worst* $O(R \cdot |A| \cdot |C| \cdot (t(m_R) + t(M_R) + t(a_R) + t(I_R))$*, where* R *is the number of rules mined by the algorithm and* $t(X)$ *is the time taken to compute function* X *from the framework.*

Proof. For a node corresponding to A' to be expanded to search for more specific rules, (for more variables to be added to it in an attempt to find larger rules), at least one rule $A' \rightarrow c : c \in C$ must have been mined, otherwise the branch of the search space is pruned. In the worst case, each child $A' \cup a : a \in (A - A')$ must be examined, with none of the rules $A' \cup a \rightarrow c : c \in C$ found to be interesting. This takes at worst $O(|A| \cdot |C|)$ time. Therefore, for each rule mined, at worst $O(|A| \cdot |C|)$ more specific but non-interesting rules may have to be examined. Finally, the processing of each rule requires one application of each of the functions m_R, M_R, a_R and I_R. □

This theorem states that the performance is linear in the number of *interesting* rules *found* by the algorithm (the number of rules for which $I_R(\cdot)$ returns *true*). *It is therefore not possible to improve the algorithm other than by a constant factor* since each interesting rule must at least be output by the algorithm. Note that this result is not the same as saying that the run time is linear in the size of the search space. The search space is known beforehand, but the required rules are not. The search space may be $O(2^{|A \cup C|})$ but if only R of these rules are interesting (and typically $R << 2^{|A \cup C|}$), then the run time of GRM is linear in R, *not* $2^{|A \cup C|}$. It is not possible to improve on the $|A| \cdot |C|$ without sacrificing completeness in a general-to-specific type algorithm. The proof of theorem 6.9 implies that the number of rules that must be examined to guarantee completeness is $O(R \cdot |A| \cdot |C|)$. The cost of garbage collection execution does not alter the complexity and the algorithm can be implemented with the same complexity without one.

Corollary 6.10. *PARM takes* $O(R \cdot |A| \cdot |C| \cdot n)$ *time. CCRules takes* $O(R \cdot |A|^2 \cdot |C| \cdot n)$ *time, where* n *is the number of samples (instances). Mining association rules with a*

Algorithm 6.1 Generalized Rule Mining (GRM) algorithm. The rules in the tree of figure 6.3 would be examined in the order: $\rightarrow a$, $\rightarrow b$, $1 \rightarrow a$, $1 \rightarrow b$, $2 \rightarrow a$, $2 \rightarrow b$, $3 \rightarrow a$, $3 \rightarrow b$, $3,1 \rightarrow a$, $3,1 \rightarrow b$, $3,2 \rightarrow a$, $3,2 \rightarrow b$, $4 \rightarrow a$, ...

class $PrefixNode\,\{PrefixNode\,parent,\ String\,name,\ double\,value_m,\ double\,value_M\}$
//node: the PrefixNode (corresponding to A') to
// expand using the vectors in joinTo.
//$x_{A'}$: the Vector corresponding to A'.

```
GRM(PrefixNode node, Vector x_A', List joinTo)
 List newJoinTo = new List();
 List currentCategory = new List();
 PrefixNode newNode = null;
 boolean addedConsequent = false;
 for each (x_v, v, lastInCategory) ∈ joinTo
  if (v ∈ C)
   double[] value_m = m_R(x_A', x_v);
   newNode = new PrefixNode(node, v, value_m, NaN);
   double[] value_M = evaluateAndSetM_R(newNode);
   if (I(value_m, value_M))
    if (M_R(·) non-trivial) store(newNode);
    outputRule(newNode);
    addedConsequent = true;
   else newNode = null;
  if (v ∈ A) //Note: possible that v ∈ A ∧ v ∈ C.
   Vector x_{A'∪v} = a_R(x_A', x_v);
   if (I_A(x_{A'∪v}))
    newNode = new PrefixNode(node, v, NaN, NaN);
  if (newNode ≠ null)
   GRM(newNode, newVector, newJoinTo);
   currentCategory.add(x_v, v, lastInCategory);
  else
   if (v ∈ C∧!addedConsequent)
    return; //prune early -- no super rules exist
  if (lastInCategory∧!currentCategory.isEmpty())
   currentCategory.last().lastInCategory = true;
   newJoinTo.addAll(currentCategory);
   currentCategory.clear();

main(File dataset)
 PrefixNode root = new PrefixNode(null, ϵ, NaN, NaN);
 Vector x_∞ = //initialise appropriately (e.g. ones)
 List joinTo = ... //read vectors from file
 GRM(root, x_∞, joinTo);
```

single variable in the consequent takes $O(R \cdot |A| \cdot |C| \cdot n)$ time. R is the number of rules mined.

Proof. For all instantiations considered in this paper, $t(m_R) = t(a_R) = O(n)$ where n is the number of samples, since all functions require examining vectors. $t(I_R) = O(1)$. For CCRules, $t(M_R) = O(|A|)$ since M_R examines immediate sub-rules. For PARM and association rule mining, $t(M_R) = O(1)$ and M_R is trivial, as sub-rules do not need to be examined due to the anti-monotonicity of support. □

The complexity of $outputRule(\cdot)$ is dependent on the application and what is done with the rules. Outputting a single rule can be done in $O(|A|)$ time, storing it in memory for later use can be done in $O(1)$ time (add operation in a hash table prevents garbage collection), finding the top k rules can be done in $O(k \log(k))$ time, etc.

Theorem 6.11. *The space usage is $O(|A \cup C| \cdot n + |A|^2)$ if M_R is trivial, and $O(R + |A \cup C| \cdot n + |A|^2)$ if M_R requires access to sub-rules[8]. Note that $O(|A \cup C| \cdot n)$ is the size of the database.*

Proof. In the worst case (all elements in A induce at least one interesting rule), all variables' vectors must remain in memory. The search is depth first, and so the depth is at most $|A|+1$. At each node along the current path of the search, a list of at most size $|A|$ is kept (containing references to objects already in memory), as well as at most one additional vector (the vector corresponding to $x_{A'}$ required to build vectors for longer antecedents). Therefore, at most $O(|A \cup C| + |A|) = O(|A \cup C|)$ vectors of length n are in memory, and $O(|A|^2)$ references to existing objects. If all mined rules need to be stored ($M_R(\cdot)$ is non-trivial), this takes $O(R)$ space at worst. □

6.6 Experiments

The primary purpose of the experiments is to demonstrate and validate the run-time complexity of the GRM algorithm and its superiority in comparison to alternative approaches. It also provides initial effectivity results for the CCRule and CMRule methods.

[8] Note that *if* the rules need to be stored, common prefixes are shared in the *Categorized Prefix Tree* and so in practice the space usage of the rules is much less than $O(R \cdot |A \cup C|)$ – at best it is $O(R)$. The worst case is only possible for trivial cases involving small R.

6.6.1 Complexity Experiments

GRM's run time is evaluated here for conjunctive rules with bit-vectors (therefore covering any counting based approach) and multiplicative rules with real valued vectors. Unfortunately, there are no existing or suitable algorithms for comparison. For example, recall that previous work on uncertain transaction databases [25, 26, 58, 7, 57] considers only itemsets, not rules. Itemset mining is very different to the *direct* mining of rules. For comparison therefore, an fast "Apriori" style method for mining rules was developed, called *FastAprioriRules*. It is based on the candidate generation and testing methodology that is common in literature. However, it mines rules directly – that is, it does *not* mine sets first and then generate rules form these as this would be inefficient. FastAprioriRules also exploits the mutual exclusion optimisation which greatly reduces the number of candidates generated, preemptively prunes by antecedents when possible and incorporates the *pruneEarly* concept. Hence FastAprioriRules evaluates exactly the same number of rules as GRM so that the comparison is fair and evaluates the characteristics of the underlying algorithms. To check if a rule matches an instance in the counting phase, a set based method is used, which proved to be much quicker than enumerating the sub-rules in an instance and using hash tree based look-up methods to find matching candidates. This is not surprising as instances in classification data sets are large. The data set is kept in memory to avoid Apriori's downsides of multiple passes, and unlike the GRM experiments, I/O time is not included. The general idea was to err on the side of giving FastAprioriRules the advantage. Two approaches were implemented using the FastAprioriRule method; a generic counting method, and PARM. Note that the latter operates on uncertain transactions.

Most rule mining methods require frequency counts. Hence, the algorithms are compared on the task of mining all conjunctive rules $A' \to c$ that are satisfied by (i.e. classify correctly) at least *minCount* instances. By varying *minCount*, the number of interesting rules mined can be plotted against the run time. The UCI [2] Mushroom and the 2006 KDD Cup data sets were used as they are relatively large. Figure 6.4(a) clearly shows the linear relationship of theorem 6.9 for *over three orders of magnitude* before the experiments were stopped (this also holds in linear-linear scale). When few rules are found, setup factors dominate. More importantly, *GRM is consistently more than two orders of magnitude faster than FastAprioriRules.* It is also very insensitive to the data set characteristics, unlike FastAprioriRules. Results on smaller data sets (UCI data sets Cleve and Heart) lead to identical conclusions and are omitted for clarity.

PARM is evaluated in a similar fashion by varying *minExpSup*. Here, the Mushroom

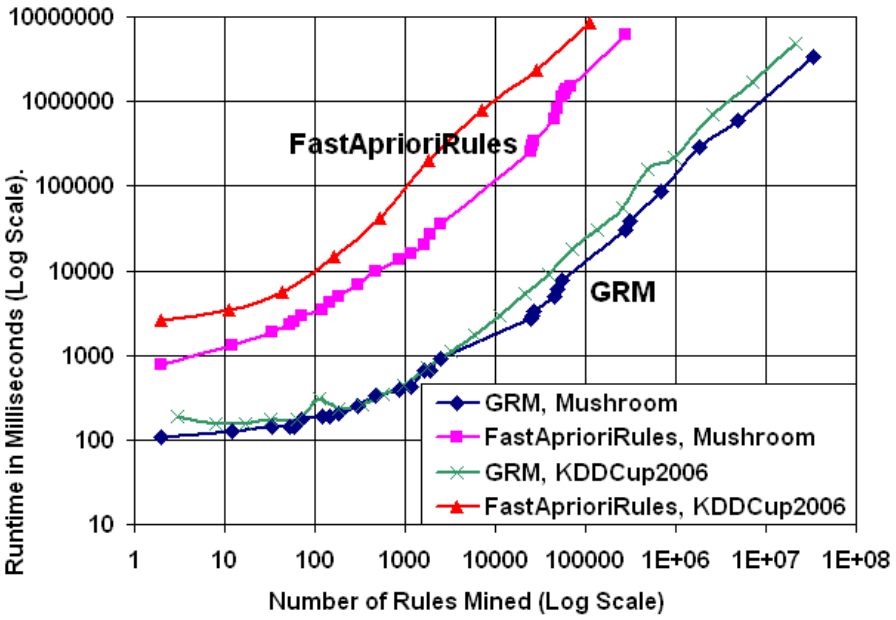


Figure 6.4: Run time comparison of support based conjunctive rules on the Mushroom data set. GRM uses bit vectors. Run-time is linear in the number of rules mined and orders of magnitude faster than FastAprioriRules. **Log-log scale**.

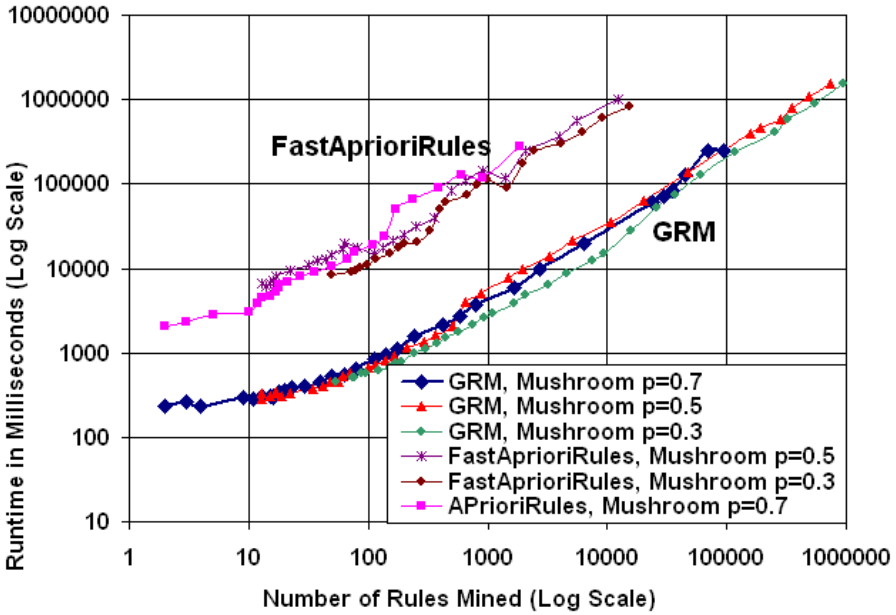


Figure 6.5: Run time comparison of PARM on three probabilistic Mushroom data sets. GRM uses real vectors. Run-time is linear in the number of rules mined and orders of magnitude faster than FastAprioriRules. **Log-log scale**.

Classifier	Breast	Cleve	Heart	Average
NaiveBayes	97.28	82.78	83.70	87.92
BayesNet	97.28	82.78	83.70	87.92
VotedPerceptron	96.28	83.11	84.07	87.82
CCRules	96.85	82.78	82.96	87.53
SPARCCC	96.14	82.78	82.22	87.05
JRip	93.56	83.11	84.44	87.04
CBA	96.30	82.80	81.90	87.00
Logistic	92.42	84.77	83.33	86.84
RandomForrest	96.28	80.13	83.70	86.71
IBk K=3	95.28	81.13	83.70	86.70
IBk K=1	95.71	79.14	81.11	85.32
Ridor	93.71	80.46	80.37	84.85
J48	94.42	74.17	82.22	83.61
Id3	90.13	76.49	82.22	82.95
PRISM	91.27	75.50	79.63	82.13
OneR	91.56	72.85	72.22	78.88

Table 6.1: Accuracy of *CCRules* used for classification.

data set was converted to a probabilistic data set by changing certain occurrences to a value chosen uniformly from $[0, 1)$ with a probability p. The resulting graph in figure 6.5(b) shows the same linear relationship for the three values of $p \in \{0.3, 0.5, 0.7\}$. Here, GRM is at least one order of magnitude faster than the FastAprioriRules implementation.

The memory footprint of GRM remained constant throughout all experiments, as expected.

6.6.2 CCRules for Classification

Three UCI [2] data sets were used for evaluating CCRules for classification, with attributes discretised using the method in [61]. $minCI$ was set to 0.05. For SPARCCC [98], the values providing the highest accuracy were used ($AggressiveS$, $SS_{p,ccr,conf}$, $p = 0.001$). For CBA, $minSup = 1\%$ and $minConf = 0.5$. All other classifiers are from WEKA with default parameters. Evaluation was via stratified 10-fold cross validation. The results in figure 6.1 clearly show that CCRules, while simple, performs well in comparison to other classifiers on these data sets, ranking 4th out of the 16 classifiers evaluated.

6.7 Conclusion

This work introduced the Generalized Rule Mining problem and solved it with the combination of a novel vectorised framework and algorithm. The usefulness of this abstraction was demonstrated by solving two very different and novel rule mining approaches. The next chapter shows a further approach. GRM was also demonstrated to be orders of magnitude faster than a fast candidate generation and testing approach on methods were this comparison is possible. Rules with novel semantics (perhaps inspired by the geometric interpretation) that are now solvable using GRM provide fertile avenues for future work.

6.8 Appendix: Notes on using Pearson's Correlation for the Evaluation of Rules

Finding rules where the antecedent and consequent are correlated with each other is intuitive, but this does not consider possible alternative consequents – perhaps one such alternative consequent is more correlated with the antecedent than the rule under consideration. This is undesirable – especially when rules are used for classification or prediction purposes such as is the case for CCRules: in a good rule, the antecedent should be more correlated with what it predicts than with the alternative(s). It turns out that this must always be the case.

Fact 6.12. *When the consequent c is binary valued, $C(A' \to c) = -C(A' \to \neg c)$. In particular, $C(A' \to c) > 0 \iff C(A' \to c) > C(A' \to \neg c)$. $\neg c$ corresponds to the consequents other than c. A' may be real valued.*

Proof. Proof that $corr(x, y) = -corr(x, \neg y)$. $||\vec{x} - \bar{\vec{x}}|| \cdot ||\vec{y} - \bar{\vec{y}}|| \cdot corr(x, y) = \sum_{i=1}^{n} x_i y_i - n\bar{x}\bar{y}$ and (1) $||\vec{x} - \bar{\vec{x}}|| \cdot ||\neg\vec{y} - \bar{\neg\vec{y}}|| \cdot corr(x, \neg y) = \sum_{i=1}^{n} x_i(\neg y)_i - n\bar{x}\bar{\neg y}$. Since y is binary valued, $(\neg y)_i = 1 - y_i$ and $\bar{\neg y} = 1 - \bar{y}$. So (1) becomes $n\bar{x} - \sum_{i=1}^{n} x_i y_i - n\bar{x} + n\bar{x}\bar{y} = -\sum_{i=1}^{n} x_i y_i + \bar{x}\bar{y} = -||\vec{x} - \bar{\vec{x}}|| \cdot ||\vec{y} - \bar{\vec{y}}|| \cdot corr(x, y)$. Note that $||\vec{y} - \bar{\vec{y}}||^2 = \sum_{i=1}^{n} y_i^2 - n\bar{y}^2$, and so $||\neg\vec{y} - \bar{\neg\vec{y}}||^2 = \sum_{i=1}^{n}(1 - y_i)^2 - n(1 - \bar{y})^2 = n - 2n\bar{y} + \sum_{i=1}^{n} y_i^2 - n + 2n\bar{y} - n\bar{y}^2 = \sum_{i=1}^{n} y_i^2 - n\bar{y}^2 = ||\vec{y} - \bar{\vec{y}}||^2$. The result follows. □

Hence, if the antecedent is positively correlated with the class variable, then the rule also has a higher correlation than the same antecedent predicting the other class(es). As a consequence, more complicated measures that may appear to be useful at first do not add any value. For example, the *class correlation difference* $CCD(A' \to c) = C(A' \to c) - C(A' \to \neg c)$ measures the difference in correlation between the rule and its alternative(s). However, by lemma 6.12, $CCD(A' \to c) = 2 \cdot C(A' \to c)$ so this measure is redundant. Similarly, if Pearson's correlation is used in a *class correlation ratio* ([98], chapter 8) then $CCR(A' \to c) = C(A' \to c)/C(A' \to \neg c) = -1$. Note however that chapter 8 uses an alternative correlation measure in defining CCR, and so is not affected by this. The lemma also provides a shortcut for mining rules for two class problems as the evaluation of a rule for one class provides the result for the other, therefore cutting the search space in half. Note that the lemma holds regardless of whether the variables in the antecedent is numeric or binary (the proof applies to the general case and would be considerably simpler in the binary case).

As far as the author is aware, previous work (e.g. [40]) has noted and used this relationship for binary valued antecedents only.

Chapter 7

Correlated Multiplication Rules with Applications to Feature Selection and Generation

Often, interactions between variables in a database are unknown to the detriment of further analysis, classification and mining tasks. This chapter proposes *Correlated Multiplication Rules* (CMRules) which capture interactions predictive of a dependent variable. CMRules are the first rules with multiplicative semantics. Furthermore, a feature selection and dimensionality reduction method is described whereby CMRules are used to generate composite features. One advantage of this approach is that it allows linear models to learn non-linear decision boundaries with respect to the original variables. Unlike other methods, the resulting features are easy to understand and initial experiments show that the proposed method can improve classification accuracy compared both to the original database and PCA projections. Finally, it is shown that the CMRule mining problem can be solved using the *Generalised Rule Mining* (GRM) framework of chapter 6.

7.1 Introduction

Feature selection and generation is an important part of the Knowledge Discovery process. This chapter proposes a data mining technique that finds rules that are able to capture interactions amongst variables that are highly correlated with a variable of interest. In contrast to other rule mining methods, the variables may be real valued or binary valued.

Rules are an important pattern in data mining due to their ease of interpretation and usefulness for prediction. They have been heavily explored as association patterns [11, 22, 81, 47, 84], "correlation" rules [22, 108] and for associative classification [61, 60, 100]. These approaches consider only conjunctions of binary valued variables – which means that the antecedent and consequent consist of a conjunction of literals that are either true or false [11, 22, 81, 47, 84, 108, 61].

Correlated Multiplication Rules (CMRules) consist of a set of real valued variables multiplied together in the antecedent, and predict a variable c in the consequent: $v_i * v_j * ... * v_k \rightarrow c$. Rules with multiplication semantics and real valued variable types are novel in the literature. CMRules find interactions between variables and are successfully used as composite features, enabling linear models to learn non-linear decision boundaries. Mixed variable types pose no problems.

Rule mining is a challenging problem due to its exponential search space in $A \cup C$, where A is the set of variables that may be in the antecedent and C is the set of variables that may be in the consequent. At best, an algorithms run time is linear in the number of interesting rules it finds, and the CMRules algorithm is provably optimal in this sense. It also scales linearly in the dimensionality of the vectors, and can use space linear in the size of the database. The algorithm uses a depth first vectorized search approach, therefore avoiding the "candidate generation" problem inherent with Apriori style algorithms.

7.1.1 Contributions

The contributions of this work are as follows:

- A new rule pattern, *Correlated Multiplication Rules* (CMRules) is introduced. It is able to find multiplicative interactions amongst features that predict a dependent variable; such as a class if used for classification. In a descriptive data mining approach, it helps find those features that interact to affect the variable being studied. Unlike other rule mining methods, it can handle real

valued data. An efficient algorithm is proposed based on the Generalised Rule Mining methodology of chapter 6.

- A feature selection, generation and reduction method is introduced whereby the antecedent of CMRules are used as composite features. This improves the fit and classification accuracy of other algorithms by explicitly allowing them to capture interactions. In particular, this enables linear models to achieve non-linear decision boundaries in the original features and thus improves the classification accuracy of such models. Since the composite features are rule antecedents, which in turn are multiplications of attributes, the approach has the advantage that the features are still interpretable. This contrasts methods like Principle Component Analysis (PCA).

7.1.2 Organisation

The remainder of this chapter is organised as follows: Section 7.2 places this work in the context of existing literature, section 7.3 presents the Correlated Multiplication Rules technique. Section 7.4 describes the method whereby CMRules can be used for composite feature generation and selection. Section 7.5 describes the CMRules algorithm. Experimental results are presented in section 7.6 and this chapter is concluded in section 7.7.

7.2 Related Work

7.2.1 Rule Mining

Most existing rule mining methods are used for associative pattern mining or classification. These only consider rules with conjunctive semantics of binary literals and use counting approaches in their algorithms. Association rule mining methods [11, 47, 81] typically mine item-sets before mining rules, rather than mining rules directly. Itemset mining methods are often extended to rule based classification, which consider one variable in the consequent [110, 61, 100]. The algorithms can be categorized into Apriori-like approaches [11] characterized by a breadth first search through the item lattice and multiple database scans, tree based approaches [47] characterized by a traversal over a pre-built compressed representation of the database, projection based approaches [100] characterised by depth first projection based searches and vertical approaches [81, 34, 96] that operate on columns. However, CMRules does not use a support based technique, requires rules rather than sets,

and most importantly; does not have conjunctive semantics and requires handling of real valued variables. Therefore, the Generalised Rule Mining (GRM) approach (chapter 6, [93]), is exploited. GRM abstracts rule mining and mines rules directly and very efficiently

7.2.2 Correlation Rules

Conjunctive rules using correlation measures have been studied in the literature, though all are quite different to those presented in this paper; [22] uses a χ^2 test to measure the significance of a correlation, but measures correlation by independence – *not* by Pearson's correlation. [108] uses Pearson's correlation, but this is applied to item pairs, not rules. FOSSIL [40] mines rules for classification using a heuristic based only on Pearson's correlation, but it is an inductive logic programming approach. While the ϕ-coefficient is often used to evaluate rules mined by other methods [88], the author is not aware of any purely correlation based approach such as *Correlation Improvement*. Furthermore, note that no previous rule mining approach applied to real valued vectors in the context of rule mining, as is done in the CMRules method.

Existing rule mining techniques are exclusively conjunctive and include association analysis and prediction or rule based classification [11, 103, 110].

7.3 Correlated Multiplication Rules (CMRules)

Linear models such as regression are important for modeling [44] and classification [104], but their power is limited by their linear decision boundary. They can be used to model non-linearities (*in terms of the original variables*) by using non-linear functions on existing variables as regressors (or 'features' in machine learning). Furthermore, when such functions are applied to multiple variables at a time, they generate *composite variables* capable of capturing non-linear *interactions* between variables. These can replace existing variables or function as additional variables in a linear model. The use of such composite variables transforms the space in which the (linear) model is built. If the composite features are non-linear in the original features, the model becomes non-linear in the *original* variables[1]. This is analogous to using kernel functions to map the space so that a non-linear decision boundary is achieved using linear models.

Good candidates for composite variables are multiplications of sets of variables. For example, the regression/decision problem $y = \alpha_1 v_1 + \alpha_2 v_2 + \alpha_3 v_3 + \alpha_{1,2} v_1 v_2 + \beta$ can

[1] Of course, it remains linear in the (composite) variables used in the model.

capture non linearities in v_1 and v_2 as well as capturing an interaction between v_1 and v_2 since it includes the term $\alpha_{1,2}v_1v_2$. Finding the right variables to multiply together in order to achieve a better fit is a challenging problem. The best composite variables are highly correlated with the dependent variable; they capture the non-linearities and interactions well and therefore allow a better fit. This is a simple but powerful idea. However, if there are m variables, there are $O(m^k)$ composite feature size to k and, in general, there are $O(2^m)$. Therefore, an intelligent search with pruning is required.

Example 7.1. Suppose we have the regression/decision problem $P : y = \alpha_1 v_1 + \alpha_2 v_2 + \beta$. We can add an extra (composite) variable v_1v_2: $P' : y = \alpha_1 v_1 + \alpha_2 v_2 + \beta + \alpha_{1,2} v_1 v_2$. This model is now capable of expressing a non-linear decision boundary in terms of v_1 and v_2 and can also capture a multiplicative interaction between v_1 and v_2. If there are no such patterns, $\alpha_{1,2}$ will be found to be 0. If there are non-linearities or interactions in the problem that can be approximated by v_1v_2 then P' will have $\alpha_{1,2} \neq 0$ and will fit better than P.

Correlated Multiplication Rules (CMRules) are rules of the form $v_i * v_j *, ..., *v_k \rightarrow c$, where the $v_i \in A$ are observed variables and c is the dependent variable to be predicted. Based on the above discussion, the antecedents of rules with the highest correlations define ideal composite variables and capture interactions explaining the dependent variable c. Furthermore, such rules are easy to interpret and understand and can therefore provide useful information to help explain interactions in the data.

The data set consists of a set of variables A and a dependent variable c. Each row in the data set consists of samples of these variables. Each column therefore contains all samples for a particular variable $v \in A$ or c. Consider these columns as vectors and denote these by x_v and x_c respectively. $x_v[i]$ is therefore the ith sample of variable v.

The CMRules presented in this chapter use Pearson's product moment correlation coefficient, although other measures can easily be used in its place. Pearson's correlation coefficient between two variables v and c may be written as

$$r_{v,c} = \frac{\sum_{i=1}^{n}(x_v[i] - \bar{x_v})(x_c[i] - \bar{x_c})}{\sqrt{\sum_{i=1}^{n}(x_v[i] - \bar{x_v})^2}\sqrt{\sum_{i=1}^{n}(x_c[i] - \bar{x_c})^2}}$$

where $r_{v,c} \in [-1, 1]$ and $\bar{x_v}$ is the mean of v. If all variables are binary valued, it reduces to the ϕ coefficient.

The correlation $C(A' \rightarrow c)$ of a rule $A' \rightarrow c$ is defined as the Pearson's product moment correlation coefficient between the antecedent and the consequent of the rule. Let the vector corresponding to the antecedent be denoted $x_{A'}$. $C(A' \rightarrow c)$ may then be written as:

$$C(A' \rightarrow c) = \frac{(x_{A'} - \bar{x_{A'}}) \cdot (x_c - \bar{x_c})}{||x_{A'} - \bar{x_{A'}}||||x_c - \bar{x_c}||}$$

Since CMRules have multiplication semantics, the vector $x_{A'}$ is defined by

$$x_{A'}[i] = \Pi_{v \in A'} x_v[i]$$

That is, for each sample / row in the database, the values of the variables in the antecedent of the rule are multiplied together. Accordingly, CMRules with a high correlation show those variables that, when multiplied together in all the samples, are highly correlated with the dependent variable c.

7.3.1 Directing the Search by Correlation Improvement

Recall that the goal is to find highly correlated CMRules. The simplest approach is to attempt to find rules with a correlation above some user defined threshold. However, it is problematic to direct the search space by only expanding rules with correlation above a threshold for two reasons.

- First, it introduces an arbitrary parameter to which the approach becomes sensitive.
- More subtly, since correlation is not downwards closed, it also introduces a dependency on the order in which variables are added to the antecedent. This could be addressed by "forcing" anti-monotonicity as a greedy heuristic but the limitation inherent in absolute threshold based techniques remains.

Instead, the following approach is used: A variable should only be added to the antecedent of a rule if it *improves* the rule compared to its generalizations. That is, if the variable improves the rule compared to those less specific rules having fewer variables in the antecedent. The *Correlation Improvement* (CI) measures this improvement in terms of correlation;

Definition 7.2. The *Correlation Improvement* is

$$CI(A' \rightarrow c) = C(A' \rightarrow c) - \max_{a \in A'}\{C(A' - \{a\} \rightarrow c)\}$$

where $A' - \{a\} \rightarrow c$ is a less specific *sub rule* obtained by removing variable a from the antecedent. Note that $A' - \{z\} \rightarrow c$ is a generalization (a less specific rule) that therefore applies to more samples, while $A' \rightarrow c$ is more specific and applies to less samples. For an empty antecedent (the base case), $CI(\emptyset \rightarrow c) = C(\emptyset \rightarrow c)$ where $x_\emptyset$ is a vector of 1s.

The *Correlation Improvement* is positive if the rule to which it is applied has a higher correlation than any of its immediate generalizations. This means it is a better predictor of the consequent variable than any of the less specific rules. This also has a geometric interpretation: Since correlation is the cosine of the angle between vectors (Recall figure 6.2), using the correlation improvement technique means the antecedent is built so that it moves closer to the consequent (in terms of the subtended angle) in comparison to the immediate sub-rules.

The following lemma shows that Correlation Improvement is downward closed.

Lemma 7.3. *If $A' \rightarrow c$ is expanded (and considered interesting) only when $CI(A' \rightarrow c) \geq 0$ then Correlation Improvement is downwards closed: If $A' \rightarrow c$ is interesting, then so are all sub-rules.*

Proof. This follows by induction over all sub-rules. □

This means that $A' \rightarrow c$ is not only more correlated than all *immediate* sub-rules, but indeed *all* sub-rules. Consequently, Correlation Improvement is a useful method to direct the search for CMRules.

It is now possible to define the CMRule problem:

Problem definition: *Correlated Multiplication Rules* (CMRules): Find all CMRules with $CI(A' \rightarrow c) > minCI$, a threshold. (Recall that A' is interpreted as a multiplication of variables; $\Pi_{v_i \in A'} v_i$).

Note that if $minCI > 0$, only variable interactions that predict the dependent variable better than all individual variables are found.

Finally, note that CMRules with a single variable in the antecedent are also useful – they can (trivially) be used to select a good subset of variables (features) to use since they simple variables that are highly correlated with the dependent variable. Recall that CMRules can be used for automated supervised variable (feature) selection and composite variable generation – in particular, for generating composite variables that allow a non-linear interactions to be captured in the model.

7.4 CMRules for Feature Selection and Generation

Recall that the antecedents of CMRules are ideal candidates for composite features, and CMRules with only a single variable in the antecedent are also useful for feature selection. This is because the interactions defined by the antecedent variables are highly correlated with the dependent variable to be predicted, and since the antecedent is the product of variables, it introduces introduces non-linearity.

In order to use CMRules for feature selection and composite feature generation, this chapter proposes the *Top Correlated Multiplication Rules (TCMR)* method as follows:

1. First, all *CMRules* are mined using the correlation improvement method.
2. Then, the rules are sorted according to their $C(A' \rightarrow c)$ values and the top ranked rules selected.
3. Finally, the antecedents of the selected rules are used as (composite) variables in the model. This means the vectors $x_{A'}$ of the selected rules $A' \rightarrow c$ become the new values of the composite features A'.

This simple procedure works well, as will be shown in section 7.6.

7.5 Mining CMRules

This chapter adopts the Generalised Rule Mining (GRM) method proposed in chapter 6. GRM is a combination of a framework of functions on vectors and an efficient algorithm for mining rules directly. It solves rule mining at the abstract level. It is used for the following reasons:

- GRM proved to be easy to apply to the problem addressed in this paper. Since GRM solves rule mining at the abstract level, the CMRules problem can be solved by instantiating the functions in the framework appropriately (below) and using the GRM algorithm.
- GRM supports real valued variables and any rule semantics. Since CMRules is the first rule based method with multiplicative semantics and real valued variables, other algorithms are not applicable.
- The GRM algorithm is efficient and uses linear time in the rules mined. It does not use "candidate generation", does not require multiple scans and does not generate a compressed version of the database.

The core of GRM is its framework, which abstracts and vectorises rule mining. Recall that A is the set of variables that may be in the antecedent, and C is the set of variables that may be in the consequent. In CMRules, $C = \{c\}$, the dependent variable to be predicted. As an aside, supposing there are multiple dependent variables, one may have $|C| > 1$. This is equivalent to mining CMRules for each dependent variable separately, however the separation method takes $O(|C|)$ times longer than if they are mined together in one go.

In the GRM framework, each possible antecedent $A' \subseteq A$ and each possible consequent $c \in C$ are expressed as vectors, denoted by $x_{A'}$ and x_c respectively. Recall that these were already defined in section 7.3. The GRM framework is composed of five functions, which can be instantiated in the following way to solve the CMRules problem:

1. $m_R : X^2 \to \mathbb{R}$ is a distance measure between the antecedent and consequent vectors $x_{A'}$ and x_c. $m_R(x_{A'}, x_c)$ evaluates the quality of the rule $A' \to c$.
   In CMRules, $m_R(x_{A'}, x_c) = C(A' \to c)$, Pearson's correlation coefficient as per section 7.3. Geometrically, in CMRules "close" means the angle between $x_{A'}$ and x_c is small (figure 6.2 on page 123).

2. $a_R : X^2 \to X$ operates on vectors of the antecedent so that $x_{A' \cup a} = a_R(x_{A'}, x_a)$ where $A' \subseteq A$ and $a \in (A - A')$. This means $a_R(\cdot)$ combines the vector $x_{A'}$ for an *existing* antecedent $A' \subseteq A$ with the vector x_a for a new antecedent element $a \in A - A'$. The resulting vector $x_{A' \cup a}$ represents the larger antecedent $A' \cup a$. Therefore, $a_R(\cdot)$ allows the antecedent vector required by $m_R(\cdot)$ to be built incrementally. Since $a_R(\cdot)$ defines how the vectors are built, it also – implicitly – defines the semantics of the rule.
   In CMRules, $a_R(\cdot)$ is the element-wise multiplication of (typically) real valued vectors: $a_R(x_{A'}, a_a)[j] = x_{A'}[j] * x_a[j]$. The semantics of CMRules are multiplicative.

3. $M_R : \mathbb{R}^{|\mathcal{P}(A')|} \to \mathbb{R}$ is a measure that evaluates a rule $A' \to c$ based on the value computed by $m_R(\cdot)$ for any sub-rule $A'' \to c : A'' \subseteq A'$. This supports interestingness measures where a rule $A' \to c$ needs to be compared with some or all of its sub-rules.
   Recall that in CMRules, the *Correlation Improvement* method ensures rules are mined that are more correlated with c than their immediate sub-rules. The *Correlation Improvement* method is implemented using $M_R(\cdot)$ according to definition 7.2.

4. $I_R : \mathbb{R}^2 \to \{true, false\}$ determines whether a rule $A' \to c$ is *interesting* based on the values produced by $m_R(\cdot)$ and $M_R(\cdot)$. Only interesting rules are output and further expanded (i.e. more specific rules are examined) by the algorithm. In CMRules, the desired search strategy is achieved when I_R returns true for $A' \to c$ if and only if $CI(A' \to c) > minCI$. Geometrically, since $C(A' \to c) = cos(\theta)$ and $CI(\cdot)$ must be positive, the search progresses by adding variables to the antecedent in a way that the antecedent vector moves closer to the consequent vector in terms of the subtended angle θ (figure 6.2 on page 123). Recall that this means variables will only be added to the antecedent if they improve the correlation with the dependent variable c in comparison to all the *immediate* sub-rules, and therefore, by lemma 7.3, all sub-rules.

5. Sometimes it is possible to determine that a rule is not interesting based purely on the antecedent. This is supported by $I_A : X \to \{true, false\}$. $I_A(x_A) = false$ implies $I_R(\cdot) = false$ for all $A' \to c : c \in C$.
   In CMRules, $I_A(x_{A'}) = true$ for all A' since it is not possible to prune the search based on the antecedent only.

With the above instantiations of the GRM framework, the GRM algorithm (algorithm 6.1 on page 132) is used to mine all CMRules efficiently.

Theorem 6.9 on page 131 gives the run time complexity of any approach that can be implemented in GRM, given the times $t(X)$ taken to compute function X in the framework.

Lemma 7.4. *Mining all CMRules takes $O(R \cdot |A|^2 \cdot |C| \cdot n)$ time, where n is the number of samples (instances) and R is the number of rules mined.*

Proof. Using theorem 6.9; $t(m_R) = t(a_R) = O(n)$ where n is the number of samples, since all functions require examining each element of the vector once. $t(I_R) = O(1)$. $t(M_R) = O(|A|)$ since M_R examines immediate sub-rules. □

This result states that the performance is linear in the number of *interesting* rules *found* by the algorithm. That is, the number of CMRules output. It is therefore not possible to improve the algorithm other than by a constant factor since each CMRule must at least be output by the algorithm. Note that this result is not the same as saying that the run time is linear in the size of the search space. The search space is known beforehand, but the required rules are not. The search space may be $O(2^{|A \cup C|})$ but if only R of these rules are interesting (and typically $R << 2^{|A \cup C|}$), then the run time is linear in R, *not* $2^{|A \cup C|}$.

Algorithm	FD_{279}	PCA_{30}	TCV_{30}	$TCMR_{30}$
Logistic	63.27	75.22	75.44	77.43
NaiveBayes	76.55	71.02	73.23	75.89
J48	76.99	68.14	74.12	74.56
VotedPerceptron	75.22	70.58	74.78	76.33
Jrip	75.22	68.58	72.79	73.67
Average	73.45	70.71	74.07	75.58

Figure 7.1: Accuracy results when *Correlated Multiplication Rules* are used as composite features. FD_{279}: Full data set of 279 real valued attributes. PCA_{30}: top 30 principle components. TCV_{30}: top 30 correlated variables ($TCMR$ limited to rules with $|A'| = 1$). $TCMR_{30}$: full $TCMR$ method.

7.6 Experiments

This section evaluates the effectiveness of CMRules when used for feature selection and generation. Run time performance of the mining algorithm is also evaluated.

7.6.1 Effectiveness

To evaluate the TCMR method, the UCI [2] Arrhythmia data set was chosen for its large number of numeric attributes. It contains 279 attributes, one class variable and 452 instances. Missing values were replaced by the attribute mean and the classes were merged into two: Arrhythmia and no Arrhythmia.

The effectiveness was tested by evaluating the classification accuracy of various classification algorithms. Experiments were performed using:

- The original data set.
- The top 30 principle components of the data set. That is, Principle Component Analysis (PCA) was performed and the the database was projected onto the 30 principle components that best captured the variance in the data set. 30 variables explained at least 95% of the variance in the database, which is why this number was chosen.
- The top 30 Top Correlated Variables (TCV). This is the TCMR method but using only those antecedents with a single variable. This functions as a feature selection (but not feature generation) method.
- The full TCMR method using the top 30 rules.

In all cases, the attributes were standardized (zero mean, unit variance). Classification accuracy was evaluated using stratified 10-fold cross validation and algorithms from WEKA [104] with default parameters, resulting in figure 7.1.

The results show a noticeable improvement using TCMR, in particular for Logistic Regression, where it improves the accuracy substantially despite using only 30 features (11% of the 279 attributes in the original data set). In fact, the TCMR and Logistic Regression combination achieved the highest classification accuracy overall. This is to be expected, as TCMR allows logistic regression to learn a non-linear decision boundary.

TCMR also consistently outperformed PCA for all classifiers. It is interesting to note that 12 out of the top 30 rules found by TCMR had multiple variables in the antecedent, demonstrating that interactions and non-linearites expressible by multiplication were present in this data set, and that multiplying variables together can improve their correlation with the dependent variable. Furthermore, only two variables that were present in a multiplication were also present as single variables, showing that CMRules can capture hidden correlations.

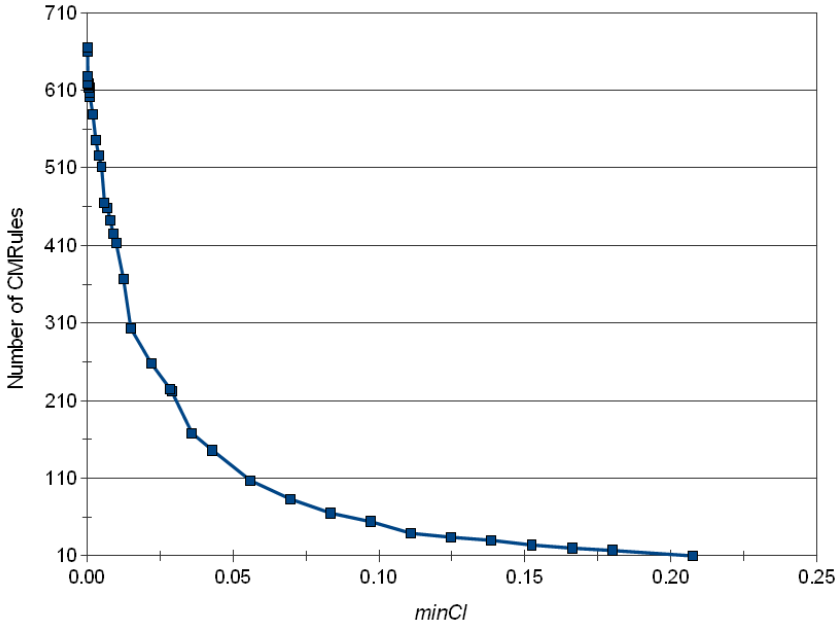


Figure 7.2: Number of CMRules mined vs *minCI* on the Arrhythmia data set.

7.6.2 Efficiency

Recall that the most difficult and computationally expensive component of the TCMR approach is the mining of the CMRules. To evaluate the run time per-

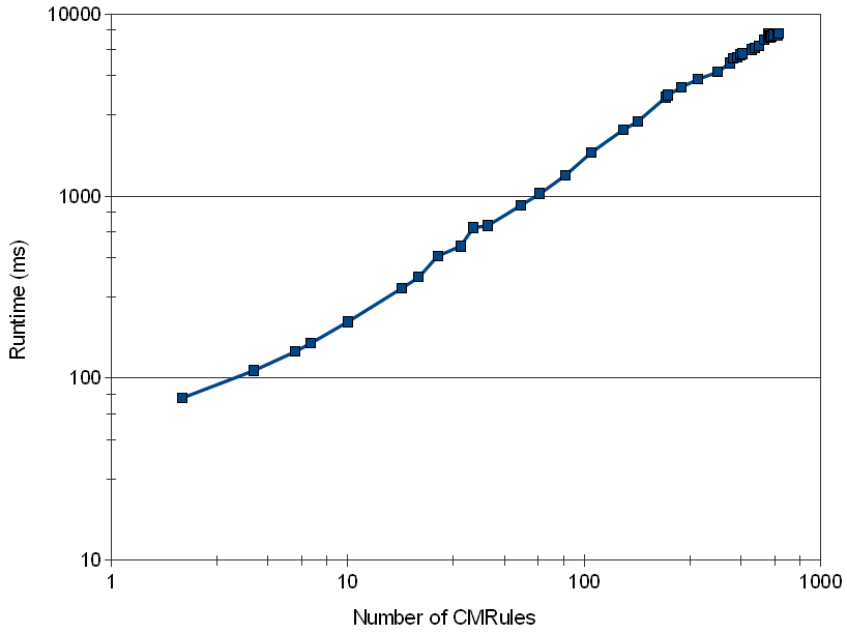


Figure 7.3: Run time in comparison to the number of rules mined on the Arrhythmia data set.

formance, the *minCI* parameter was varied and all CMRules mined that setting. Figure 7.2 shows the number of rules mined for various *minCI* settings. Figure 7.3 shows the run time in comparison to the number of rules mined in log-log scale. Above about the first 10 rules, it is clear to see that the run time is linear in the number of rules mined.

7.7 Conclusion

Often, interactions between variables in a database are unknown to the detriment of further analysis, classification and mining tasks. This paper proposed *Correlated Multiplication Rules* (CMRules) which are able to capture interactions predictive of a dependent variable. CMRules are the first rules with multiplicative semantics and are applied to feature selection and dimensionality reduction. This method uses CMRules to generate composite features, enabling linear models to learn non-linear decision boundaries with respect to the original variables. The resulting features are easy to understand and initial experiments showed that the proposed method can improve classification accuracy compared both to the original database and PCA projections. Finally, it is shown that the CMRule mining problem can be solved efficiently using the *Generalised Rule Mining* (GRM) framework.

Part III

Statistical Data Mining Methods

Chapter 8

Using Significant, Positively Associated and Relatively Class Correlated Rules for Classification of Imbalanced Databases

The application of association rule mining to classification has led to a new family of classifiers which are often referred to as Associative Classifiers (ACs). The advantage of using rule based approaches is that they are easy to interpret and perform a global search, compared to many other rule based approaches that use a greedy search strategy.

Rule-based classifiers can play an important role in applications such as medical diagnosis and fraud detection where data sets are almost always imbalanced. The focus of this chapter is to extend ACs for classification on imbalanced data sets using statistics based techniques.

This work combines the use of statistically significant rules with a new measure, the Class Correlation Ratio (CCR), to build an AC called SPARCCC. A detailed set of experiments show that in terms of classification quality, SPARCCC performs comparably on balanced data sets and greatly outperforms other AC techniques on imbalanced data sets. It also has a significantly smaller rule base and is more computationally efficient than traditional support-confidence based associative classifiers.

8.1 Introduction

Since the introduction of CBA [61] many variations on Associative Classifiers (ACs) have been proposed in the literature [60, 13, 110, 100, 28, 30, 15, 89]. Most of the ACs are based on rules discovered using the *support-confidence* paradigm and the classifier itself is a collection of rules ranked using confidence or variation thereof. In many application domains, the data sets are imbalanced, i.e., the proportion of samples from one class is much smaller than the other class(es). Additionally, the smaller class is the class of interest. For example; fraud detection and medical diagnoses. Unfortunately, the *support-confidence* framework does not perform well in such cases.

Many of the rules mined using *support-confidence* are spurious and are irregularities in the data rather than properties of the underlying population or process, motivating the statistically significant rules proposed by Webb [103]. The same holds true of rules used for classification. It is also well known that confidence has non-intuitive properties in imbalanced data sets. For example, high confidence rules can also be negatively correlated. This chapter combines statistically significant rules with a new measure, the *Class Correlation Ratio* (CCR), which leads to a better classifier. Furthermore, the proposed method does *not* use the support-confidence paradigm.

8.1.1 Contributions

This chapter makes the following contributions:

- It proposes the *Class Correlation Ratio (CCR)*, which measures the relative class correlation of a rule. A high CCR is desirable because it means the rule is more positively correlated with the class it predicts than the alternative(s). CCR also forms the basis of an effective rule ranking method that does not require confidence.
- It proves that confidence and support are biased toward the majority class in imbalanced data sets in the context of CCR. This result also motivates a correction for confidence's bias, and is a key component in making the classifier perform well on both balanced and imbalanced data sets.
- An associative classifier is proposed that is based on statistical techniques. The method is called *Significant, Positively Associated and Relatively Class Corre-*

lated Classification (SPARCCC) because it uses only rules that are statistically significant and positively associated, and where the antecedent is more correlated with the class it predicts than with the other class(es). It also searches directly for significant rules and uses this to prune the search space. SPARCCC outperforms *support-confidence* based associative classifiers on balanced data sets in terms of computational performance, and on imbalanced data sets in both computational and classification performance. SPARCCC is parameter-free, in the sense that it does not use thresholds – except standard levels of significance – to prune rules. Finally, since the rules are statistically significant and relatively class correlated, they may be examined for insights into the data.

8.1.2 Organisation

The the remainder of this chapter is organised as follows: Section 8.2 gives a brief background in associative classification. Section 8.3 describes the *class correlation ratio* and the significance test used. Section 8.4 proves that confidence (and support) are biased against the minority class under CCR. Section 8.5 describes the SPARCCC technique. Section 8.7 contains experimental results. Related work is surveyed in section 8.8 and this chapter concludes in section 8.9.

8.2 Background: Associative Classification

8.2.1 Association Rule Mining

In Association Rule Mining (ARM), the data is a set of transactions $T = \{t_1, ..., t_{|T|}\}$, each of which is a subset of the set of items: $t_i \subseteq I$, $I = \{i_1, ..., i_{|I|}\}$. The *support* of an *itemset* $X \subseteq I$ is $sup(X) = |\{t_i : X \subseteq t_i \wedge t_i \in T\}|$. An association rule $X \rightarrow Y$ is an implication between two mutually exclusive itemsets X and Y. The *support* of $X \rightarrow Y$ is $sup(X \rightarrow Y) = sup(X \cup Y)$ and its $confidence$, an *estimate* of the probability that Y occurs given that X occurs, is $conf(X \rightarrow Y) = sup(X \rightarrow Y)/sup(X)$.

8.2.2 Associative Classification

This chapter assumes a discrete data set D with attributes $A = \{a_1, a_2, ..., a_{|A|}\}$, one of which is the class attribute a_c. In every instance $d \in D$, each attribute $a_i \in A$ takes one of a finite number of possible values $V_i = \{v_{i,1}, ..., v_{i,|V_i|}\}$ so that $d = [v_{1,j}, v_{2,k}, ..., v_{|A|,l}]$ (for some $j, k, ..., l$). As an ARM task, the attribute-value

pairs become items (Namely, $i_{|V_1|+...+|V_{i-1}|+j} \equiv (a_i = v_{i,j})$) and the instances become corresponding transactions. The previous instance d then becomes a transaction $t = \{(a_1 = v_{1,i}), (a_2 = v_{2,j}), ..., (a_{|A|} = v_{|A|,k})\}$. Clearly, there will be $\sum_{i=1}^{|A|} |V_i| = |I|$ items and each transaction will have size $|A|$. Since the described mapping is a bijection, one can freely interchange *instances* and *transactions* when convenient.

8.2.3 Associative Classification Rule Mining

The Associative Classification Rule Mining (ACRM) task is to find *interesting* rules $X \rightarrow y$ where X is a set of *legal* (an attribute cannot occur more than once) attribute-value pairs and y is one of the class attribute-value pairs. "*Interesting*" rules are rules that, in conjunction with other mined rules, are likely to perform well for classification of unseen data.

8.3 Significance and Class Correlation Ratio for Rules

8.3.1 Fisher's Exact Test

There are strong arguments for mining statistically significant rules [103]. These also hold true when the rules are used for classification, as one would like to make a decision based on significant evidence.

Support is often used as a measure of "significance", the reasoning being that rules that have high support are "intuitively" more likely to capture the underlying process generating the data, rather than being artifacts of the data set or generated by noise. However, this is simply not the case and one can easily generate counterexamples showing insignificant high support or significant low support rules.

This work considers rules $X \rightarrow y$ that are statistically significant in the positively associated direction. Toward that end, Fisher's Exact Test (FET) is used on contingency tables of the form of figure 8.1[1].

[1]Statistical tests on such tables determine whether there is a significant association between the variables, compared to the null hypothesis of no association. If the sampling scheme is such that only the total (n) is fixed (or it is unrestricted), then the null hypothesis is that the variables are independent of each other, in the sense that the probability of falling into a particular row is independent of the column a particular subject is in, and vice versa (This symmetry means that the tests give the same result for $[a, b; c, d]$ as they do for $[a, c; b, d]$.) [31]. For example, $P(V_1, V_2) = P(V_1) \cdot P(V_2)$. Statistical tests compute the probability (the p-value) of obtaining a table at least as unusual as the observed table. If the p-value is below a level of significance, then there is assumed to be sufficient evidence to reject the null hypothesis and therefore we can say with some confidence level that the variables are correlated.

FET is an *exact test* (*permutation test*) that computes the p-value of an observed contingency table by explicitly calculating the probability of different table configurations, rather than using an approximate or limiting distribution. This work uses the positive one sided FET to test whether rules are significant in the positive direction. Given a table $[a, b; c, d]$, FET will find the probability (p-value) of obtaining the given table or a table where X and y are more *positively associated* under the null hypothesis that $\{X, \neg X\}$ and $\{y, \neg y\}$ are independent, and that the margin sums are fixed. The p-value is given by:

$$p([a, b; c, d]) = \sum_{i=0}^{\min(b,c)} \frac{(a+b)!(c+d)!(a+c)!(b+d)!}{n!(a+i)!(b-i)!(c-i)!(d+i)!}$$

Only rules whose p-values are below the level of significance desired are used, as they are statistically significant in the positively associated direction.

FET's continuous approximation – the χ^2 test – could also be used, but since it is a two sided test it cannot distinguish positive associations and is thus less desirable.

8.3.2 Correlation (Interest Factor)

Correlation also forms an important component of the technique in this work. This chapter proposes that rules $X \to y$ should be used when X is more positively correlated with y than it is with $\neg y$. The following definition of correlation[2] is used:

$$\hat{corr}(X \to y) = \frac{sup(X \cup y) \cdot |D|}{sup(X) \cdot sup(y)} = \frac{a \cdot n}{(a+c) \cdot (a+b)}$$

X and y are positively (negatively) correlated if $\hat{corr}(X \to y) > 1$ (< 1), and independent otherwise. Note that $\hat{corr}(X \to y) = I(X, y)$, where $I(X, y)$ is the *Interest Factor* [88]. This measure has downsides when used by itself. It is clear to see that increasing the size of the data set by increasing d (refer to figure 8.1) will increase the correlation between X and y – even though it is actually increasing the association between $\neg X$ and $\neg y$. The reverse holds for decreasing d.

Example 8.1. Consider the table $T_1 = [100, 20; 20, 10]$ where X and y are have a strong association but $\hat{corr}(X \to y) = 1.04$ (almost independent). If d is increased to get $T_2 = [100, 20; 20, 200]$, then clearly $\neg X$ and $\neg y$ are strongly associated, but $\hat{corr}(\neg X \to \neg y) = 1.4$ while now $\hat{corr}(X \to y) = 2.36$. This is clearly undesirable.

[2] To be more precise, $\hat{corr}(X \to y)$ this is the *estimate* of $corr(X \to y) = \frac{P(X \cup y \subseteq t)}{P(X \subset t) \cdot P(y \in t)}$, where $corr(X \to y)$ is defined over the underlying process that generates the data.

This problem arises only in imbalanced data sets; note that changing d alters the class distribution.

Therefore, SPARCCC does not search for positively correlated rules using $\hat{corr}$. When a rule is described as being positively associated or correlated, the author means using the *one sided* test of significance using FET. FET does not have the downside described above because of the constant margin sum restriction. Indeed, $p(T_1) = 0.041$ (significant at the 0.05 level) and $p(T_2) = 1.07 \cdot 10^{-44}$ (highly significant).

8.3.3 Class Correlation Ratio

SPARCCC uses $\hat{corr}(\cdot)$ to measure how correlated X is with y *compared* to $\neg y$ using the proposed *Class Correlation Ratio (CCR)*:

Definition 8.2. The *Class Correlation Ratio (CCR) is defined as:*

$$CCR(X \to y) = \frac{\hat{corr}(X \to y)}{\hat{corr}(X \to \neg y)} = \frac{a \cdot (b+d)}{b \cdot (a+c)}$$

The CCR measures how much more positively the antecedent is correlated with the class it predicts, relative to the alternative class(es). This avoids the downsides of using an absolute correlation measure – indeed, terms cancel out. Furthermore, intuitively one would not want to use a rule that is more correlated with classes other than the one it predicts!

Example 8.3. Returning to Example 8.1, $CCR(X \to y) = 1.25$ for T_1 and $CCR(X \to y) = 9.17$ for T_2. This also says that $X \to y$ is a better rule under T_2 than under T_1. This is true – it is much more discriminative because under T_1, y is already the majority class and therefore the rule does not provide much additional information. In fact, the information gain of using $X \to y$ over $\emptyset \to y$ is only 0.072 bits under T_1 but is 0.215 bits under T_2. Recall also that the rule was much more significant under T_2.

SPARCCC uses only rules with $CCR > 1$, so that no rules are used that are more positively associated with the classes they do not predict. Furthermore, CCR is also used in the *strength score* – which used to rank rules for classification – in order to correct for the bias of confidence. This will be covered shortly.

	X	$\neg X$	Σrows
y	a	b	$a+b$
$\neg y$	c	d	$c+d$
Σcols	$a+c$	$b+d$	$n=a+b+c+d$

$\equiv [a, b; c, d]$

Figure 8.1: 2×2 Contingency Table for $X \rightarrow y$. The notation $[a, b; c, d]$ will often be used as shorthand in the text.

Statement...	...about sample (data set) *estimate* for lemma 8.5.
A	$sup(y) < sup(\neg y)$
B	$CCR(X \rightarrow y) > 1$
B'	$CCR(X \rightarrow y) < 1$
C	$conf(X \rightarrow y) > conf(X \rightarrow \neg y) \equiv sup(X \rightarrow y) > sup(X \rightarrow \neg y)$
C'	$conf(X \rightarrow y) < conf(X \rightarrow \neg y) \equiv sup(X \rightarrow y) < sup(X \rightarrow \neg y)$

Figure 8.2: Statements for lemma 8.5. $\neg y$ means all class attribute-values other than y.

8.4 Relative Correlation Bias of Confidence (and Support) on Imbalanced Data sets

Confidence is widely used as a measure of strength of a classification rule $X \rightarrow y$ because it is an *estimate* (the data set is a sample) of the probability that, given the attribute-value pairs in X appear in an instance d generated by the underlying process, the instance will have the class label y. That is, $conf(X \rightarrow y) \approx P(y \in d | X \subset d)$. The confidence of a significant rule is therefore a useful measure of the rule strength in classification – but only in balanced data sets. In the following, it is shown that confidence (and support) are biased toward the majority class under the CCR. This result is useful for explaining why using confidence to rank rules for classification of imbalanced data sets can give poor performance. It also provides additional reasons to use CCR for ranking rules. Section 8.5.1 describes a method that attempts to correct for the bias.

Example 8.4. Note that in Example 8.1, $conf(X \rightarrow y) = 0.83$ in both T_1 and T_2 despite the rule being clearly better in T_2.

Lemma 8.5. *Confidence (and support) are biased toward the majority class under the* Class Correlation Ratio. *Specifically (statements in parentheses are defined in*

figure 8.2):

1. *If $X \to y$ is more positively correlated than $X \to \neg y$ but has a lower confidence (support), then y must be the minority class: $(B \wedge C' \implies A)$.*
2. *If $X \to y$ is more positively correlated and more confident (frequent) than $X \to \neg y$, we cannot say anything about whether y is the minority or majority class: $(B \wedge C \not\implies A$ and $B \wedge C \not\implies \neg A)$.*
3. *If y is the minority class and $X \to y$ is more confident (frequent) than $X \to \neg y$, then it is also more positively correlated: $(A \wedge C \implies B)$.*
4. *If y is the minority class and $X \to y$ is less confident (frequent) than $X \to \neg y$, there is no relationship between the correlation of the rules: $(A \wedge C' \not\implies B$ and $A \wedge C' \not\implies \neg B)$.*
5. *If y is the minority class and $X \to y$ is less positively correlated than $X \to \neg y$, it is also less confident (frequent): $(A \wedge B' \implies C')$.*
6. *If y is the minority class and $X \to y$ is more positively correlated than $X \to \neg y$, then we cannot say anything about their confidences (supports): $(A \wedge B \not\implies C'$ and $A \wedge B \not\implies \neg C')$.*

Proof. For each corresponding statement:

1. $C' \implies 1 > sup(X \cup y)/sup(X \cup \neg y)$,$B \implies sup(X \cup y)/sup(X \cup \neg y) > sup(y)/sup(\neg y)$, hence $B \wedge C' \implies A$.
2. Counter examples: If $sup(y) = 0.3 \cdot n = n - sup(\neg y)$, $sup(X) = 0.5 \cdot n$, $sup(X \cup y) = 0.3 \cdot n$ and $sup(X \cup \neg y) = 0.2 \cdot n$, a contradiction is obtained for $B \wedge C \implies \neg A$. If $sup(y) = 0.7 \cdot n = n - sup(y)$, $sup(X) = 0.8 \cdot n$, $sup(X \cup y) = 0.6 \cdot n$ and $sup(X \cup \neg y) = 0.2 \cdot n$, a contradiction is obtained for $B \wedge C \implies A$.
3. $C \implies \frac{sup(X \cup y) \cdot n}{sup(X) \cdot sup(y)} > \frac{sup(X \cup \neg y) \cdot n}{sup(X) \cdot sup(\neg y)} \cdot \frac{sup(\neg y)}{sup(y)}$, which, using A, is greater than $\frac{sup(X \cup \neg y) \cdot n}{sup(X) \cdot sup(\neg y)} = corr(X \to \neg y)$.
4. Counter examples: Let $sup(y) = 0.3 \cdot n = n - sup(\neg y)$.
   (a) If $sup(X \cup y) = 0.2 \cdot n$ and $sup(X \cup \neg y) = 0.3 \cdot n$ and $sup(X) = 0.5 \cdot n$ contradicts $A \wedge C \not\implies \neg B$.

(b) If $sup(X \cup y) = 0.2 \cdot n$ and $sup(X \cup \neg y) = 0.6 \cdot n$ and $sup(X) = 0.8 \cdot n$ contradicts $A \wedge C' /\!\!\Longrightarrow B$.

5. $B' \implies \frac{sup(X \cup y)}{sup(X)} < \frac{sup(X \cup \neg y)}{sup(X)} \cdot \frac{sup(y)}{sup(\neg y)}$, which, using A, is less than $\frac{sup(X \cup \neg y)}{sup(X)} = conf(X \rightarrow y)$.

6. Counter examples: Let $sup(y) = 0.3 \cdot n = n - sup(\neg y)$ and $sup(X) = 0.5 \cdot n$. If $sup(X \cup y) = 0.2 \cdot n$ and $sup(X \cup \neg y) = 0.3 \cdot n$, a contradiction is obtained for $A \wedge B \implies \neg C'$. If $sup(X \cup y) = 0.3 \cdot n$ and $sup(X \cup \neg y) = 0.2 \cdot n$, a contradiction is obtained for $A \wedge B \implies C'$.

□

Suppose the user has a two class problem and y describes the minority class. 3) says that if $X \rightarrow y$ is more confident than $X \rightarrow \neg y$, then it is also more positively correlated. However, the reverse does not hold as described by 4). That is, if $X \rightarrow \neg y$ is more confident than $X \rightarrow y$, then it may or may not be more positively correlated. This means that using support or confidence, the user may receive a highly confident rule for the majority class, $X \rightarrow \neg y$ (that is more confident than $X \rightarrow y$), but is actually less positively correlated than $X \rightarrow y$ – this is very undesirable! In the opposite case, 5) says that a rule in the minority class, $X \rightarrow y$, with lower relative correlation will also have lower confidence than $X \rightarrow \neg y$. Again, this does not hold for the majority class. *Since higher confidence (support) for a rule in the minority class implies higher relative correlation ($CCR > 1$), and lower relative correlation ($CCR < 1$) in the minority class implies lower confidence, but neither of these are true for the majority class, confidence (support) tends to bias the majority class. This is because confidence (support) and CCR can only 'contradict' each other in the majority class.*

In a related matter, 1) says that if $X \rightarrow y$ is more positively correlated than $X \rightarrow \neg y$ but is less confident, then y must be the minority class. Again, the reverse does not hold in general. *Hence, if a user chooses high confidence (support) rules, they are more likely to miss rules that have $CCR > 1$ applying to the minority class than in the majority class. Furthermore, when ranking by confidence (support), a user is likely to use rules with $CCR < 1$ predicting the majority class over rules with $CCR > 1$ predicting the minority class.*

Example 8.6. Consider an imbalanced data set with $sup(y) = 15$ and $sup(\neg y) = 100$. A possible contingency table is $[5, 10; 10, 90]$. Despite $conf(X \rightarrow y) = \frac{1}{3} < conf(X \rightarrow \neg y) = \frac{2}{3}$, X has a significant positive association with y ($p_{value} = 0.02$).

Also, $corr(X \rightarrow y) = 2.56$ and $corr(X \rightarrow \neg y) = 0.77$ so this rule has a high CCR ($CCR = 3.32 >> 1$) and is thus a very good rule at distinguishing between classes.

8.5 SPARCCC

There are four components to SPARCCC. How they fit together is briefly described here, and the subsequent sections outline them in detail.

1. The *Interestingness and Rule Ranking* technique (section 8.5.1) determines which of the *potentially interesting* rules mined by the *search and pruning strategy* (see below) are in fact *interesting*. It also assigns them a *strength score*, which is later used to rank the rules according to their expected usefulness in making a classification decision.

2. The *search and pruning strategy* (section 8.5.2) determines how the space of all possible rules is examined and pruned. This determines the candidate rules – the *potentially interesting* rules. The choice of strategy determines the computational performance and this chapter evaluates three possibilities.

3. The *rule selection method* (section 8.5.3) determines which of the *interesting* rules are to be used for classification. It makes use of the *rule ranking* strategy and outputs *selected* rules.

4. The *classification method* (section 8.5.4) determines how an unseen instance is classified by using the *selected* rules. It makes use of the *rule ranking* strategy and influences the *rule selection* algorithm.

8.5.1 Interestingness and Rule Ranking

8.5.1.1 Interestingness

SPARCCC performs the following tests to determine whether a *potentially interesting* rule is *interesting*:

- It checks the significance of a rule $X \rightarrow y$ by performing FET on the contingency table of figure 8.1 and records the p_{value}. The rule is significant if $p_{value} < significanceLevel$, a specified level of significance. This ensures that the rule is not a spurious relationship and that it is positively associated.

- It checks whether $CCR(X \rightarrow y) > 1$. If this is not the case, the rule is not interesting because it is more correlated with the alternative class(es) than it is with the class it predicts.

The *interesting* rules – those that pass the above two tests – are candidates for the classification task.

8.5.1.2 Rule Ranking

In order to use the rules to make a classification, a ranking (ordering) is required that captures the ability of the rule to make a correct classification. This ordering is defined by the *Strength Score (SS)* of the rule: $SS(X \rightarrow y)$. Based on the discussions in sections **8.3** the following is used as the strength score:

$$SS_{p,CCR}(X \rightarrow y) = (1 - p_{value}) \cdot CCR(X \rightarrow y)$$

Confidence is an estimate of the probability that, given X occurs, y will occur. Therefore in balanced data sets, choosing the rule with the highest confidence gives the highest expected probability of making a correct classification. For comparison therefore, the following strength score is also evaluated:

$$SS_{p,conf}(X \rightarrow y) = (1 - p_{value}) \cdot conf(X \rightarrow y)$$

However, as lemma 8.5 showed, confidence has a bias toward the majority class. While $SS_{p,conf}$ performs well on balanced data sets, it performs very poorly on imbalanced data sets. Recall that a) a highly confident rule predicting the majority class may in fact be more negatively correlated than the same rule predicting the other class(es), and b) a rule that is more positively correlated but predicts the minority class may have much lower confidence than the same rule predicting the other class(es). The interestingness criteria above excludes case a), but it does not correct for the bias in confidence for less extreme cases and it does nothing to fix case b). Therefore, this chapter suggests that this can be corrected using CCR:

$$SS_{p,conf,CCR}(X \rightarrow y) = (1 - p_{value}) \cdot conf(X \rightarrow y) \cdot CCR(X \rightarrow y)$$

This works by giving poor rules a lower score (in comparison to better rules) and scaling up cases of b): $CCR(X \rightarrow y) > 1$. In terms of a suitable classification

performance $P(\cdot)$, experiments show that on relatively balanced data sets:

$$P(SS_{p,CCR}) \approx P(SS_{p,conf,CCR}) \approx P(SS_{p,conf})$$

While on imbalanced data sets (as would be expected):

$$P(SS_{p,CCR}) >> P(SS_{p,conf,CCR}) >> P(SS_{p,conf})$$

That is, the use of CCR achieves the highest performance on imbalanced data sets while performing comparably on balanced data sets. As expected, this agrees nicely with the discussions and theoretical results in sections 8.3 and 8.4. Furthermore, note that in a completely balanced data set, $CCR(X \to y)$ reduces to $\frac{sup(X \to y)}{sup(X \to \neg y)} = \frac{conf(X \to y)}{conf(X \to \neg y)}$ which shall be called the *Class Support Ratio* and the *Class Confidence Ratio* respectively. Effectively, the more imbalanced the data set, the higher the effect of CCR. Finally, note that the p_{value} has little impact in the final score, because it varies at most by the significance level. It's inclusion therefore favors more significant rules only if the other components of SS are similar. Based on both the theory and the experimental results, the author recommends the use of $SS_{p,c,CCR}$.

Example 8.7. Recall Example 8.6 where a highly positively correlated and significant rule had a very low confidence of $\frac{1}{3}$, so $SS_{p,conf} = 0.33$. However, $CCR(X \to y) = \frac{2.56}{0.77} = 3.33$. Inclusion of this in the strength score raises it from 0.33 to $SS_{p,conf,CCR} = 0.33 \cdot 3.33 = 1.09$. In comparison, if the classes had been equally distributed, the rule would have been negatively correlated, insignificant and $CCR(X \to y)$ would have been $\frac{1}{2}$. This demonstrates how CCR can be used to counteract the bias of $conf(\cdot)$ in imbalanced data sets. Clearly, $SS_{p,CCR} = 3.27$.

8.5.2 Search and Pruning Strategies

This section describes the techniques used to prune the search space for classification rules. The overall strategy is a bottom up enumeration technique, as all the less specific rules $X' \to y : X' \subset X$ will be examined before a more specific rule $X \to y$ is generated and examined. The underlying algorithm used to perform this search is beyond the scope of this chapter. A number of approaches may be applied, however, the author recommends the use of GRM (chapter 6) due to its space and run time advantages.

The idea of a rule being statistically significant is not anti-monotonic. To avoid examining all rules, search strategies are used that ensure the concept of being *potentially*

	$t:X \subset t$	$t:X-\{z\} \subset t \wedge z \notin t$	$t:X-\{z\} \subset t$
$t:y \in t$	a	b	$a+b$
$t:\neg y \in t$	c	d	$c+d$
	$a+c$	$b+d$	$a+b+c+d$

In terms of *support*:

	$t:X \subset t$	$t:X-\{z\} \subset t \wedge z \notin t$	$t:X-\{z\} \subset t$
$t:y \in t$	$sup(X \rightarrow y)$	$sup(X-\{z\} \rightarrow y) - sup(X \rightarrow y)$	$sup(X-\{z\} \rightarrow y)$
$t:\neg y \in t$	$sup(X \rightarrow \neg y)$	$sup(X-\{z\} \rightarrow \neg y) - sup(X \rightarrow \neg y)$	$sup(X-\{z\} \rightarrow \neg y)$
	$sup(X)$	$sup(X-\{z\}) - sup(X)$	$sup(X-\{z\})$

Figure 8.3: The contingency table $[a, b; c, d]$ used to test for the significance of the rule $X \rightarrow y$ in comparison to *one* of its generalizations $X-\{z\} \rightarrow y$ for the **Aggressive-S** search strategy. The entries in the tables are the transactions satisfying the conditions.

interesting is anti-monotonic – i.e. $X \rightarrow y$ might be considered as potentially interesting if and only if all $\{X' \rightarrow y | X' \subset X\}$ have been found to be potentially interesting: The author believes that "forcing" measures that are related to classification performance to have a property they do not naturally have is better than using a measure (such as support) that has the property, but is not related to classifier performance.

The following search strategies are used to mine potentially interesting rules:

- Select a new attribute-value in such a way that it makes a significant positive contribution to the rule, when compared to all *immediate* generalizations. Specifically, figure 8.3 describes how to test for the significance of the rule $X \rightarrow y$ in comparison to *one* of its generalizations $X-\{z\} \rightarrow y$. The rule $X \rightarrow y$ is potentially interesting only if the test passes for all immediate generalizations $\{X-\{z\} \rightarrow y : z \in X\}$. This technique prunes the search space most aggressively, as it performs $|X|$ tests per rule. However, this also means that it greatly favors shorter rules, as they have fewer tests to pass. This approach is borrowed from Webb [103]. It is called **Aggressive-S** in this chapter.

- Use FET as described in section 8.3 and force it to be anti-monotonic[3]. This strategy is called **Simple-S**. It performs one test per rule and examines more

[3]That is, if and only if all rules $\{X-\{z\} \rightarrow y : z \in X\}$ are *potentially interesting*, then the contingency table of figure 8.1 is used to determine whether $X \rightarrow y$ is *potentially interesting*. Note that this is recursive.

of the search space.

- For comparison, a minimum support threshold strategy is also used. All rules with $supp(X \rightarrow y) \geq minSup$ are *potentially interesting*. This strategy is called **Support** in the experiments.

For *Aggressive-S* and *simple-S*, define $sup(\emptyset) = |D|$ so that it is possible to evaluate a p_{value} (usually high) for so-called "default rules" – rules with no antecedent that can be applied when no other rules match an instance.

8.5.3 Rule Selection Method

The rule selection algorithm (algorithm 8.1) returns the set of highest ranking rules so that each training instance is covered by (and correctly classified by) enough rules for it to have *minGroups* groups of rules, where each group is made up of rules with the same scores. This is a type of covering technique. The concept of groups is required by the classification method used.

8.5.4 Classification Method

The classification algorithm (algorithm 8.2) classifies an unseen instance based on the highest ranked (according to the strength score) matching rules. If there is one rule with the highest score, or multiple rules with the same score but predicting the same class, then the choice is straightforward – simply pick the class predicted by the rules. However, if there are multiple rules with the same score but predicting different classes, then the class is picked that is predicted by the majority of the rules in the group. In cases where there is no single majority, first remove from consideration any classes that are not in the majority. Then, the next group of rules is used to make a decision between the remaining classes. This process is continued until there is a majority in a group. If the rules run out, a random choice is made between the *remaining* classes[4].

[4]SPARCCC ensures that it does not make a decision due to running out of rules for any of these classes. For example, suppose there are 3 matching rules, and further suppose there are two rules predicting different classes in the top group. It is not possible to make a decision based on the top group alone. Hence, the next group is considered. Suppose a decision were to be made based on the single remaining rule even though the other class is not represented in this group (recall the rules for it have run out, and there was a higher ranked rule for that class in the previous group). Note also that the single rule used may have a very low score. This were to create a bias toward the class that has the most rules, even if they are of poor quality. This is not fair to the class for which fewer rules were found (for whatever reason – for example, this could happen if it was the minority class). So in this case, a random choice is made in place of relying on left over rules. Indeed, it

Algorithm 8.1 Rule selection algorithm for SPARCCC.

```
// R is the set of rules found
// T is the set of training instances (transactions)
SR = ruleSelectionByGroups(R,minGroups)
  sort R in descending order by the rule's score (r.score)
  SR = ∅ // the selected rules
  for each t ∈ T
    prevScore = ∞, groups = 0
    for each r ∈ R and while groups < minGroups
      if (r.X ⊆ t.X ∧ r.y == t.y)
        // the rule applies to and correctly classifies t
        SR = SR ∪ r
        if (r.score < prevScore)
          groups++
          prevScore = r.score
  return SR
```

Recall that the rule selection pruning algorithm ensures that there are at most *minGroups* groups of rules with the same score for each training instance. Therefore, one can expect to have up to *minGroups* groups to base a decision on when classifying. In practice, *minGroups* can be set low since the top group is often enough. $minGroups = 3$ was used in this work.

8.5.5 A Note on Interpreting the Rules

Since the proposed method performs many tests of significance, it is not possible to say that a particular rule is statistically significant because of the multiple tests problem [3]. Since each rule has a (low) chance of occurring by chance alone (at most the level of significance), one could find a significant rule by chance simply by testing rules until one is found. This is not a problem for the classification task because a set of rules is being used, rather than a particular rule. However, the multiple tests problem must be kept in mind if an attempt is made to interpret the rules as part of knowledge discovery.

was found that making a prediction based solely on the class that has the majority of rules (i.e.: ignoring the score) can have poor performance. In practice, when testing this on a few data sets, the random choice was never exercised.

Algorithm 8.2 Classification algorithm for SPARCCC.

// t is an instance to classify
// SR is the set of selected rules.
$c =$ **classifyByGroups**(t)
  $M = \{r | r.X \subseteq t \wedge r \in SR\}$ *// the matching rules.*
  $C = \{r.y | r \in M\}$ *// classes predicted by matching rules.*
  $min = \min_c |\{r.y == c \wedge r \in M\}|$
    //the minimum number of matching rules for a class.
  $min = min \cdot |C|$ *// the number of rules we can use without*
    // running out of rules for any class
  keep the first min rules in M when sorted in descending
    order by $r.score$ and delete the rest
  group the rules in M by equal score
  $counts[|C|] = [0, ..., 0]$
  for each group g, from highest to lowest score
    for each $c \in C$
      $counts[c] += |\{r | r \in g \wedge r.y == c\}|$
        // the number of rules in g predicting c
    $max = max_{c \in C}\{counts[c]\}$
    for each $c \in C$
      if $(counts[c] < max)$ *// not a majority.*
        $C = C - c$
    if $(|C| == 1)$ *// have one standout majority class*
      return the only $c \in C$
  return a randomly chosen $c \in C$.

8.6 Mining SPARCCC Rules using GRM

The *search and pruning strategy* (rule mining) part of SPARCCC can be implemented in GRM as follows. Note that the terminology of chapter 6 is used, with rules $A' \rightarrow c$ instead of the $X \rightarrow y$ notation used in thie chapter.

- The database is the set of vectors corresponding to individual variables, $D = \{x_v : v \in A \cup C\}$, where A is the set of attribute-value pairs and C is the set of classes. $x_a[i] = 1 : a \in A$ if the attribute-value pair a is present in the ith instance. Similarly, $x_c[i] = 1 : c \in C$ if the ith instance has class c. In all other cases, the ith entry of the vectors is 0.

- $m_R(x_{A'}, x_c)$ calculates the contingency table $[n_{11}, n_{10}, n_{01}, n_{00}]$ (figure 6.1), as described in section 6.4. This corresponds to the contingency table $[a, c, b, d]$

of figure 8.1 in this chapter (note the different order due the different table headings). $n_{11} = x_{A'} \cdot x_c$; the dot-product of the two vectors. Note that this is the number of instances in which the rule $A' \rightarrow c$ holds (it's support). $n_{10} = |x_{A'}| - n_{11}$, $n_{01} = |x_c| - n_{11}$ and n_{00} can be calculated as $n - n_{11} - n_{01} - n_{10}$ where n is the length of the vectors. From this, it can calculate the p value (p_{value}) of the rule, it's CCR and it's confidence ($conf$) as described in this chapter. Let the result of $m_R(\cdot)$ evaluated on the rule $A' \rightarrow c$ be the array $value_m(A' \rightarrow c) = [n_{11}, n_{10}, n_{01}, n_{00}, p_{value}, CCR, conf]$. For simplicity, let the notation $value_m(A' \rightarrow c).n_{11}$ refer to the n_{11} entry, etc.

- $a_R(x_{A'}, x_a)$ is defined so that $x_{A' \cup a}[i] = x_{A'}[i]\, AND\, x_a[i]$. Hence, $x_{A' \cup a}[i] = 1$ if the antecedent $A' \cup a$ matches the ith instance.

- $M_R(\cdot)$ is defined differently, depending on the search and pruning strategy used.

  - For **Agressive-S**, it must evaluate the significance of $A' \rightarrow c$ in comparison to all the rule's immediate generalisations. The contingency table $[a, b, c, d]$ of figure 8.3 can be obtained as follows: $a = value_m(A' \rightarrow c).n_{11}$, $b = value_m(A' - x \rightarrow c).n_{11} - a$ (where $A' - z \rightarrow c$ is a subrule of $A' \rightarrow c$ obtained by removing $z \in A'$), $c = value_m(A' \rightarrow c).n_{10}$ (the number of instances supporting the rule $A' \rightarrow \neg c$), and $d = value_m(A' - z \rightarrow c).n_{10} - c$. By constructing this table for all immediate sub-rules and testing the significance as described in this chapter, $M_R(\cdot)$ can determine whether the $A' \rightarrow c$ significantly improves on it's immediate generalisations. Let $AggresiveS.p_{value}$ be the maximum p_{value} of all these tests. Of course, the computation can be aborted early one any of the tests deliver an insignificant p_{value}, in which case set $AggresiveS.p_{value} = 1$.
  - For **Simple-S**, $M(\cdot)$ must check to see if $A' \rightarrow c$ as well as all it's immediate sub-rules are significant as determined by the significance test implemented in $m_R(\cdot)$. Let $SimpleS.p_{value} = \max\{value_m(A' \rightarrow c).p_{value}, \max_{z \in A'}(value_m(A' - z \rightarrow c).p_{value})\}$.
  - For **Support,** $M(\cdot)$ is trivial.

- $I_R(\cdot)$ determines which rules are interesting and should be expanded. Again, this is determined by the strategy used:

  - For **Agressive-S**, $I_R(\cdot)$ returns true if and only if $AggresiveS.p_{value} < significanceLevel$.
  - For **Simple-S**, $I_R(\cdot)$ returns true if and only if $SimpleS.p_{value} < significanceLevel$.

  - For **Support**, $I_R(\cdot)$ returns true if and only if $value_m.n_{11} \geq minSup$.

- $I_A(\cdot)$ can only be exploited in the **Support** method, in which case it returns false if $|x_{A'}| \leq minSup$. In all other methods, $I_A(\cdot)$ is always *true*.

The above instantiation of GRM efficiently mines all *potentially interesting* rules. It also calculates all the values required by the *interestingness and rule ranking* strategy.

8.7 Experiments

Experiments were performed[5] on relatively balanced well known UCI data sets [65] as well as imbalanced variations of them. The data sets used were {Australia, breast, Cleve, Diabetes, Heart, Horse}[6].

In the tables, the proposed methods are denoted by "SPARCCC" with the search strategy in parentheses. For comparison, a purely support and confidence based technique was also used, denoted by "Support-Confidence". It finds all rules satisfying the support and confidence thresholds and uses confidence as the strength score[7]. Any techniques using a support based search (such as CBA and CMAR) have *exactly* the same search space (and *at least* the same run time) as "Support-Confidence". Hence these are not reported separately.

8.7.1 Original (Balanced) Data sets

This section presents experiments on the original data sets, where the class distributions are roughly balanced. Figure 8.4 shows that (on average) SPARCCC performs comparably to CBA, CMAR and C4.5[8], and is insensitive to the choice of SS. However, there are large differences in the search space examined and hence the run times, as shown in figures 8.6(a) and 8.6(b). Also, much fewer rules are found as can be seen in figure 8.6(d). Despite having very similar accuracy, the search space explored by "Aggressive-S" is $\{1.6\%, 1.4\%, 1.3\%\}$ (for significances of $\{0.05, 0.01, 0.001\}$ respectively) of that explored using a support based technique with $minSup = 1\%$[9]. For the less aggressively pruned search, "Simple-S", it is $\{18.9\%, 10\%, 6\%\}$.

[5] The experiments were performed on an laptop with: Intel Pentium M 2.0GHz, 1GB of RAM, Windows XP Professional. Programs written in Java. Stratified 10-fold cross validation was used for measuring all performance indicators.

[6] Continuous variables were discretised using the technique of [61]

[7] That is, there is no use of significance tests or correlation at all. The rule selection and classification procedure is as described in this paper.

[8] The reported accuracy levels for C4.5, CBA and CMAR were obtained from [60].

[9] It should be noted that $minSup = 1\%$ is usually recommended. $minSup = 5\%$ performs worse, and as will be shown, is terrible on skewed data sets.

Algorithm	*Strength Score*	*minSup*	*minConf*	*significance*	*Australia*	*Breast*	*Cleve*	*Diabetes*	*Heart*	*Horse*	*Average*
SPARCCC (Aggressive-S)	$SS_{p.conf.CCR}$	na	na	0.05	84.1	95.6	81.1	77.0	81.1	73.0	**82.0**
		na	na	0.01	84.5	96.1	81.5	77.3	80.7	78.4	**83.1**
		na	na	0.001	84.2	96.1	82.8	78.0	82.2	78.4	**83.6**
	$SS_{p.conf}$	na	na	0.05	85.8	94.3	82.1	75.0	81.9	75.4	**82.4**
		na	na	0.01	86.4	95.1	82.1	73.7	80.0	80.3	**82.9**
		na	na	0.001	85.9	95.3	83.4	71.5	82.6	80.1	**83.1**
	$SS_{p.CCR}$	na	na	0.05	84.1	95.4	81.8	77.1	81.1	72.4	**82.0**
		na	na	0.01	84.2	96.0	81.8	76.3	81.1	78.4	**83.0**
		na	na	0.001	84.2	96.0	83.1	76.3	82.2	78.4	**83.4**
SPARCCC (Simple-S)	$SS_{p.conf.CCR}$	na	na	0.05	83.3	95.7	82.8	77.6	83.0	75.7	**83.0**
		na	na	0.01	83.5	95.9	82.1	77.6	83.0	75.7	**82.9**
		na	na	0.001	85.1	95.0	82.8	77.1	83.0	74.6	**82.9**
	$SS_{p.CCR}$	na	na	0.05	83.6	95.7	82.8	78.0	83.0	75.4	**83.1**
		na	na	0.01	83.2	95.9	82.1	78.0	83.0	75.4	**82.9**
		na	na	0.001	85.1	95.1	82.8	77.9	83.0	74.3	**83.0**
SPARCCC (Support)	$SS_{p.conf.CCR}$	1%	na	0.05	84.2	95.7	82.1	76.7	81.9	78.4	**83.2**
		5%	na	0.05	84.6	93.3	81.8	77.5	83.0	79.0	**83.2**
	$SS_{p.CCR}$	1%	na	0.05	84.3	95.7	81.8	76.6	82.2	77.0	**82.9**
		5%	na	0.05	85.5	92.7	82.1	73.0	83.3	80.1	**82.8**
Support-Confidence	conf	1%	0.5	na	85.4	95.6	82.8	76.7	83.3	80.3	**84.0**
		5%	0.5	na	85.5	92.7	81.8	73.0	83.0	80.1	**82.7**
CBA	na	1%	0.5	na	84.9	96.3	82.8	74.5	81.9	82.1	**83.8**
CMAR	na	1%	0.5	na	86.1	96.4	82.2	75.8	82.2	82.6	**84.2**
C4.5	na	na	na	na	84.7	95.0	78.2	74.2	80.8	82.6	**82.6**

Figure 8.4: Accuracy on original data sets.

Algorithm	Strength Score	minSup	minConf	significance	Australia	Breast	Cleve	Diabetes	Heart	Horse	Average
SPARCCC (Aggressive-S)	$SS_{p,conf,CCR}$	na	na	0.05	53.5	88.2	31.6	19.6	23.5	30.8	**41.2**
		na	na	0.01	48.8	90.2	5.3	19.6	11.8	19.2	**32.5**
		na	na	0.001	32.6	82.4	0.0	5.4	0.0	19.2	**23.2**
	$SS_{p,conf}$	na	na	0.05	2.3	68.6	0.0	0.0	0.0	0.0	**11.8**
		na	na	0.01	2.3	70.6	0.0	0.0	0.0	0.0	**12.2**
		na	na	0.001	0.0	56.9	0.0	0.0	0.0	0.0	**9.5**
	$SS_{p,CCR}$	na	na	0.05	69.8	88.2	42.1	46.4	47.1	30.8	**54.1**
		na	na	0.01	74.4	90.2	31.6	44.6	17.6	42.3	**50.1**
		na	na	0.001	58.1	86.3	26.3	39.3	5.9	46.2	**43.7**
SPARCCC (Simple-S)	$SS_{p,conf,CCR}$	na	na	0.05	41.9	74.5	42.1	32.1	41.2	26.9	**43.1**
		na	na	0.01	39.5	78.4	31.6	33.9	23.5	26.9	**39.0**
		na	na	0.001	39.5	76.5	5.3	17.9	0.0	19.2	**26.4**
	$SS_{p,CCR}$	na	na	0.05	41.9	74.5	42.1	55.4	41.2	26.9	**47.0**
		na	na	0.01	39.5	80.4	31.6	55.4	35.3	26.9	**44.8**
		na	na	0.001	39.5	80.4	21.1	39.3	11.8	34.6	**37.8**
SPARCCC (Support)	$SS_{p,conf,CCR}$	1%	na	0.05	58.1	70.6	31.6	23.2	29.4	42.3	**42.5**
		5%	na	0.05	23.3	0.0	0.0	0.0	0.0	7.7	**5.2**
	$SS_{p,conf}$	1%	na	0.05	58.1	52.9	21.1	0.0	23.5	42.3	**33.0**
		5%	na	0.05	23.3	0.0	0.0	0.0	0.0	3.8	**4.5**
	$SS_{p,CCR}$	1%	na	0.05	58.1	70.6	31.6	42.9	29.4	42.3	**45.8**
		5%	na	0.05	25.6	17.6	5.3	0.0	11.8	7.7	**11.3**
Support-Confidence	conf	1%	0.5	na	14.0	37.3	5.3	0.0	11.8	0.0	**11.4**
		5%	0.5	na	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
CBA	na	1%	0.5	na	79.3	59.2	18.5	36.3	0.0	29.0	**37.1**
CCCS	na	na	na	na	64.2	74.3	27.8	30.9	18.7	41.6	**42.9**

Figure 8.5: True positive rate (recall, sensitivity) of the minority class on imbalanced versions of the data sets.

Algorithm	minSup	minConf	significance	Australia	Breast	Cleve	Diabetes	Heart	Horse	Average
SPARCCC (Aggressive-S)	na	na	0.05	2,840	4,805	1,251	874	3,361	29,023	7,026
	na	na	0.01	2,089	4,102	929	724	1,921	27,831	6,266
	na	na	0.001	1,525	3,404	661	519	1,436	25,894	5,573
SPARCCC (Simple-S)	na	na	0.05	168,762	55,149	16,520	3,136	47,105	210,735	83,568
	na	na	0.01	102,804	35,854	14,047	2,680	47,105	61,749	44,040
	na	na	0.001	55,218	23,532	11,376	2,136	47,057	19,347	26,444
any Support method	1%	any	any	501,939	10,527	71,038	8,363	321,577	1,733,455	441,150
	5%	any	any	38,095	2,202	11,460	2,454	72,060	19,152	24,237

(a) Search space size on original datasets

Algorithm	minSup	minConf	significance	Australia	Breast	Cleve	Diabetes	Heart	Horse	Average
SPARCCC (Aggressive-S)	na	na	0.05	0.184	0.125	0.067	0.073	0.062	0.106	0.103
	na	na	0.01	0.135	0.112	0.050	0.057	0.056	0.070	0.080
	na	na	0.001	0.115	0.100	0.043	0.057	0.045	0.060	0.070
SPARCCC (Simple-S)	na	na	0.05	17.024	1.281	0.917	0.557	3.909	13.556	6.207
	na	na	0.01	10.239	0.954	0.756	0.484	3.911	4.732	3.513
	na	na	0.001	4.587	0.740	0.575	0.410	3.870	1.474	1.943
any Support method	1%	any	any	116.873	3.850	6.795	1.190	30.917	353.708	85.556
	5%	any	any	3.284	0.822	0.700	0.379	5.198	1.076	1.910

(b) Training time on original datasets

Algorithm	minSup	minConf	significance	Australia	Breast	Cleve	Diabetes	Heart	Horse	Average
SPARCCC (Aggressive-S)	na	na	0.05	1,877	3,272	424	238	420	2,341	1,429
	na	na	0.01	1,318	2,762	309	194	293	1,459	1,056
	na	na	0.001	1,072	1,951	246	170	232	736	735
SPARCCC (Simple-S)	na	na	0.05	89,496	31,416	8,865	3,336	25,815	24,771	30,617
	na	na	0.01	54,738	23,382	5,213	2,705	22,617	5,043	18,950
	na	na	0.001	31,670	15,125	2,986	1,813	17,889	1,289	11,795
any Support	1%	any	any / na	501,132	10,701	93,387	7,314	270,694	2,080,527	493,959
	5%	any	any / na	50,843	3,152	13,355	2,534	67,169	39,039	29,349

(c) Search space size on imbalanced versions of the datasets.

Algorithm	minSup	minConf	significance	Australia	Breast	Cleve	Diabetes	Heart	Horse	Average
SPARCCC (Aggressive-S)	na	na	0.05	172	128	128	48	113	101	115
	na	na	0.01	107	105	85	39	85	50	79
	na	na	0.001	66	85	56	29	59	35	55
SPARCCC (Simple-S)	na	na	0.05	39,653	5,375	5,028	1,104	16,384	36,059	17,267
	na	na	0.01	21,061	3,669	4,181	908	16,384	9,250	9,242
	na	na	0.001	8,455	2,461	3,144	710	16,336	2,723	5,638
SPARCCC (Support)	1%	na	0.05	182,996	5,094	19,926	2,762	69,187	344,860	104,138
	5%	na	0.05	15,708	1,090	4,760	896	29,326	6,339	9,687
any Support-Confidence	1%	0.5	na	218,637	5,175	31,091	3,415	137,545	772,506	194,728
	5%	0.5	na	15,953	1,091	4,932	965	31,164	7,065	10,195

(d) Number of rules found (prior to rule selection) on the original datasets.

Figure 8.6: Computational performance on original and imbalanced data sets.

*So, picking the best accuracy (*83.6%*, "Aggressive-S" using significance of* 0.001 *and* $SS_{p,conf,CCR}$*) SPARCCC can obtain comparable accuracy while searching only 1.3% of the space, using 0.08% of the time and finding 0.03% of the rules, when compared to support based methods – for example; CBA and CMAR.*

8.7.2 Imbalanced Data sets

Highly imbalanced versions of the data sets were obtained by keeping the majority class and randomly selecting a subset of the minority class so that the ratio was

1 : 9. That is, the percentage of instances with the minority class was 10%. Figure 8.5 shows the True Positive Rate (TPR) of the minority class. Note that accuracy is a poor performance measure for imbalanced data sets because one can obtain high (at least 90%) accuracy by predicting the majority class. TPR (also known as sensitivity and recall) is a much better performance indicator. The accuracy is therefore not shown for space reasons. It remains high however.

The effect of using CCR in the SS is large. One can clearly see the following relationship:

$$TPR(SS_{p,CCR}) >> TPR(SS_{p,conf,CCR}) >> TPR(SS_{p,conf})$$

For example, *when using "Aggressive-S",* $SS_{p,conf,CCR}$ *is on average (over data sets and significance levels)* 2.87 *times better than* $SS_{p,conf}$ *and* $SS_{p,CCR}$ *is* 1.58 *times better than* $SS_{p,conf,CCR}$ *and* 4.44 *times better than* $SS_{p,conf}$. A similar, though slightly smaller effect occurs for "Simple-S" and "Support-S".

The proposed methods also score much higher than other rule based techniques such as CBA and CCCS, the latter of which was designed specifically for imbalanced data sets. The highest average TPR overall is for "Aggressive-S" with a significance level of 0.05. This was 45.8% better than CBA and 26.1% better than CCCS. Unlike for the original data sets, the significance level has a large impact on the classification performance on imbalanced data sets, likely due to the pruning of the search space. Interestingly, the use of CCR had the unexpected benefit of reducing this effect. It was also noticed that much fewer rules were generated overall. Finally, the computational performance favors the proposed techniques even more on imbalanced data sets. Figure 8.6(c) for example shows that "Aggressive-S", at a significance level of 0.05, explores only 0.29% of the space considered by a support based method with $minSup = 1\%$ – and the training time is even less. For "Simple-S" it is 6.2%. Note also that the performance of any support based technique with $minSup = 5\%$ is very poor, as is to be expected on such an imbalanced data set.

Overall, the experiments show that, by using SPARCCC with a significance based search strategy, one can achieve much better classification performance on skewed data sets than techniques such as CBA (which is outperformed it by up to 45.8% when using a significance level of 0.05) while using dramatically fewer computational resources (0.29% of those used by support based methods).

8.8 Related Work

CBA [61] was the first Associative Classifier (AC) proposed and most other ACs are variations on the original CBA design which consists of three components: 1) rule mining, 2) rule selection (classifier building) and 3) classification. For *rule mining*, CBA mines all rules passing support and confidence thresholds ($minSup$ and $minConf$). Additionally, it ignores rules based on a "pessimistic error based pruning method" borrowed from C4.5 [76]. Unfortunately, $minSup$ and $minConf$ need to be set very low for decent accuracy, generating tens of thousands of rules – most of which perform poorly. Therefore, a *rule selection* process is needed to select a small subset likely to perform well. Rules are selected so that each training instance is covered by the highest ranked rule that matches the instance, and each rule, when considered together with the others, will be used to correctly classify at least one training instance. New instances are *classified* according to the highest ranked rule that is applicable. Rules are ranked according to confidence, support, and size.

CMAR [60] has many similarities to CBA. The main differences[10] are the use of a χ^2 test instead of the error based pruning and a more complicated classification procedure involving an empirically chosen weighted χ^2 measure applied to multiple matching rules. CMAR uses the same contingency table (figure 8.1) as one of the interestingness criteria proposed in this chapter. However, the χ^2 test does not distinguish between directions of association and therefore the claim in [60] that only positively correlated rules are found is not necessarily correct. Negatively associated rules are just as likely to pass the test as positively associated ones. For example, the table $[4, 25; 12, 15]$ is significant at the 0.05 level but X is negatively associated (correlated) with y. Though CMAR checks for significance, it is still based on the *support-confidence* framework.

In general, rules with $CCR(\cdot) < 1$ will incorrectly classify the training data. The above techniques still work because, in balanced data sets, choosing high support and confidence rules tends to favor positively correlated rules, but this is *not* the case in imbalanced data sets as lemma 8.5 shows.

CBA, CMAR and related techniques rely heavily on support and confidence for searching, pruning and ranking rules. While popular and convenient, there is little evidence to suggest they are any good at finding useful classification rules. Indeed, both CMAR and CBA need to use $minSup = 1\%$ and $minConf = 0.5$ in their

[10] We note that CBA is based on the Apriori algorithm, while CMAR is based on FP-Growth. Such differences do not change the rules that are found, just the way in which they are found, and hence are irrelevant for this discussion.

experiments to beat C4.5 [61, 60], generating tens of thousands of rules. Note that CMAR's χ^2 test, CBA's error rate pruning and the use of confidence does not reduce the search space. A large number of rules found, many of which are poor, dictates the requirement of often complex rule selection methods. It is not uncommon for these to discard 99% of the mined rules [61, 60] – meaning the search by support and confidence has an effective precision of only 1%.

It is not surprising then, that techniques using the *support-confidence* framework perform poorly on imbalanced data sets. The approach in this chapter is much simpler: the rule mining method finds statistically significant and positively associated rules. Since the number of rules found is typically very small, and SPARCCC directly mines for rules that are expected to perform well for classification, there is no need for rule selection. SPARCCC has a very simple classification method; a simple strength score is used to rank the rules and the highest ranked matching rule is used. This straightforward technique performs comparably on balanced data sets, much better on imbalanced data sets and has greatly reduced computational requirements.

The CCCS [15] technique was proposed to find positively correlated rules. It takes into account imbalanced class distributions, enabling it to outperform other techniques on imbalanced data sets while performing competitively on balanced data sets. Another upside is that it is relatively parameter free. It does not rely on support to prune the search space, but instead forces *correlation* to be locally monotonic and uses a *top down row enumeration* algorithm. However, there is no guarantee that the rules found are statistically significant, and this algorithm generates many thousands of rules. It is also very computationally intensive an does not scale well for traditional data sets where there are more instances than attributes.

Morishita et al. [63] use the same test as CMAR but find upper-bounds on χ^2 for search space pruning. It is an association rule mining technique and is not used for classification.

Webb [103] proposed the use of Fisher's Exact Test (FET) to examine the significance of association rules in more detail than [60, 63]. The technique is used in the *Aggressive-S* search strategy employed in this chapter for pruning the search space. Webb does not use the rules for classification – instead it is used for knowledge discovery. This requires consideration of the issue of multiple tests. Since the mined rules are not validated, it is very difficult to determine whether the rules are useful. This chapter mines significant rules under a number of different strategies and uses them for classification – which also requires additional work such as rule selection, ranking and classification. This gives a very good performance indicator – performance on unseen data in comparison to other algorithms. As a side effect, the

author believes that this also provides extra weight to the method proposed in [103].

8.9 Conclusion

The traditional measures of support and confidence are fundamental in association rule mining and associative classifiers. However, they have many downsides, especially when used for classification of imbalanced data sets. Many rules found under such schemes are statistically insignificant, negatively correlated, the antecedent and consequent are independent of each other, or the antecedent is more positively correlated with the alternate classes than the class it predicts. Furthermore, in imbalanced data sets these measures favor the majority class, and in this chapter this was proved in the context of the Class Correlation Ratio. If this is not corrected, classification performance suffers. There is also little evidence that support is good for anything other than pruning the search space, and even then, it must be set to very low values in order to capture useful rules. However, at this point many thousands of rules can be generated – most of which will be discarded (sometimes even 99% [60]). The author believes this support and confidence approach is inefficient and that there is an over-reliance on these measures for historical or simplicity reasons.

This chapter makes the case that searching directly for significant rules is more appropriate. From a theoretical standpoint, it makes sense to use statistically significant and positively correlated rules, and additionally require that they are more positively correlated with the class they predict than with the alternatives. This has been validated by experiments on the novel associative classifier introduced in this chapter – SPARCCC. The experiments showed similar classification performance on balanced data sets, and higher classification performance on imbalanced data sets compared to other ACs. Furthermore, by searching directly for significant rules, SPARCCC is faster as it does not need to explore as much of the search space. Finally, it also uses much fewer rules, suggesting that it is much better at finding quality predictive rules.

The author feels that this work lends some weight to the argument that it is better to focus on measures that are statistically sound and are linked to classifier performance, and if necessary, force these to be anti-monotonic for computational efficiency – than to use approaches which are not directly related to classifier accuracy but have an inherent anti-monotonic property.

Chapter 9

Mining Complex Sub-graphs of Correlated Variables with Applications to Feature Selection

Finding interactions between variables is a fundamental concept in Data Mining. This chapter considers correlations between variables using Pearson's product moment correlation coefficient and mines *complex, complete,* and *maximal* sub-graphs describing the correlation structure between variables. Both positive and negative (complex) correlations are considered. It is proved that under a constraint on the minimum level of correlation desired, there are useful guarantees on the graph's structure; the sign of the correlation between vertices can be mapped to the vertices themselves, leading to *complex sets*. Therefore, complex interactions become simpler to understand and a novel algorithm is presented that mines complex interactions in the same run time as if negative correlations were not considered.
The approach is useful for examining complex correlation structures in databases and mining representative subsets. The latter idea is extended to a feature subset selection method that gives guarantees on the minimum correlation required for features to be considered interchangeable (redundant), while guaranteeing that the selected features are not correlated with each other. Experiments show the approach performs well.

9.1 Introduction

Finding interactions between variables is a fundamental concept in Data Mining. This chapter investigates the correlation structure between variables. In the graph view, each variable is a vertex, and an edge exists between vertices if the magnitude of the correlation between the corresponding variables exceeds a threshold. Graphs defined by a *lack* of correlation are also briefly considered. The sign of the correlation (positive or negative) is taken into account and the edge labeled accordingly.

In this work, *completely connected* sub-graphs (cliques) are of interest because these guarantee that every variable in the sub-graph is highly correlated with each other variable, therefore describing a strong symmetric relationship. An application of this structure is to use one variable in place of the variables in the sub-graph. Being completely connected is useful here; the user may define a level of correlation over which the variables are considered to be equivalent – or more precisely; of insufficient difference to warrant inclusion of more than one of them. This is the basis for applying the approach to feature subset selection in section 9.5.

It is important to consider both positive and negative correlations – that is, "complex" sub-graphs. If only positive or high magnitude correlations are considered, much of the structure will be missed as negative correlations will not be included. For example, A may be highly correlated with D, but both of these may also be negatively correlated with B and C. This methods in this chapter mine complete and complex sub-graphs capturing such a structure. The goal is to represent these as *complex sets* of variables – sets of variables that may include negated variables – that are all highly positively correlated with each other. For instance, the complex set $\{A, -B, -C, D\}$ indicates that A, $-B$ (negative B), $-C$ and D are highly *positively* correlated, describing the above-mentioned pattern. Without consideration for complex relationships, either a) two separate sets $\{A, B\}$ and $\{C, D\}$ would be mined instead or b) the set $\{A, B, C, D\}$ would be mined – in both cases failing to show the complete structure of the interaction.

This chapter shows that under a practical constraint on the correlation coefficient, mining complex sub-graphs can be reduced to mining complex sets of variables, as a majority of the edge combinations are impossible. Furthermore, the positive and negative labeling of variables in the sets can be achieved for free. This achieves significant computational savings and makes complex interaction patterns easier to understand: Suppose there is a complete sub-graph G' on the variables $V' \subseteq V$, where V is the set of all variables. There are $|V'|^2/2$ edges in G' and therefore $2^{|V'|^2/2}$ possible labellings of edges as either positive or negative. Hence, there are

$2^{|V'|^2/2}$ different complex correlation structures. The results in this chapter show that under the constraint, only $2^{|V'|}$ of these are possible. This is precisely the number of labellings of vertices in G', which means that instead of mining and reporting entire sub-graphs including edge labels – and incurring the correspondingly higher complexity – the same problem can be solved by mining *complex sets* of variables. Furthermore, of the $2^{|V'|}$ possibilities, half are the negation of all variables in another combination, leaving $2^{|V'|-1}$ configurations. Finally, it will be shown that the labellings can be achieved for free using the proposed algorithm: searching through all possible subsets of all vertices V takes $O(2^{|V|})$ time, but the algorithm also labels the variables within this time. Therefore, the results in this chapter reduce the complexity of the problem from $O(2^{|V'|^2/2})$ to $O(2^{|V'|})$.

Since mining these complex sets creates the problem of redundancy (each set of size k will contain $2^k - 1$ subsets), this work focuses on mining *maximal* sets (maximal complete sub-graphs).

9.1.1 Motivations

Each maximal complex set of variables indicates that all the variables in that set are highly positively correlated with every other variable. Furthermore, no other variable (or its negation) can be added to the set without breaking this property. Such correlation structures are interesting in their own right and can indicate near duplicate variables or flag previously unknown complex interactions. By comparison, analysing or graphing a correlation matrix usually hides interactions that involve more than two variables at a time.

Each maximal complex set can also be thought of as capturing an underlying feature, or "factor", in the process captured by the data set. Of course, there are other approaches for doing this, namely Principle Component Analysis (PCA) [44], Singular Value Decomposition (SVD) – which is related to PCA – and Factor Analysis [44] – which uses PCA. In these approaches, each principle component capture a source of variability in the data – that is, a factor. While it is possible to examine the coefficients of a principle component in order to determine what variables are associated with it, it is a technique that does not provide the type of guarantees on the correlation structure that the approach in this chapter does. It also becomes difficult to do when many variables are involved. The advantages of the proposed technique are that it gives guarantees on the correlations in a set, it maintains the actual variables (unlike PCA), and the resulting patterns are easy to interpret.

A concrete application of this idea is to provide suggestions for selecting a represen-

tative set of features. It is therefore applied to the problem of *feature subset selection* [88] using a three stage *filter* [88] approach: First, maximal complex sets of variables (features) are mined. The variables in such a set are considered interchangeable, as they are highly correlated with each other. Then, a representative variable for each set is found, taking account the overlap between other sets. This is intended to remove from consideration any redundant, duplicate, or otherwise unnecessary variables while capturing the primary factors in the underlying process. Finally, a subset of the representative variables is chosen so that none of them are correlated with each other.

The approach allows the user to define the minimal correlation required for features to be considered interchangeable, and provides a guarantee that the features selected will not be correlated. Another advantage is that a *subset* of the original features are used as selected features. This means models such as trees and rules built on these remain highly interpretable, contrasting approaches such as PCA or SVD which produce features that are linear combinations of *all* original features. Linear combinations as features make the resulting models very difficult to interpret. Furthermore, they do not reduce the number of attributes that need to be collected in future: The principle components are only orthogonal if the linear combination is not truncated. This means that while the algorithm uses fewer features, the features used are still a function of all the original features.

9.1.2 Contributions

This chapter makes the following contributions:

- *Complete, complex and maximal sub-graphs (sets)* of correlated variables are proposed as useful patterns for describing complicated correlation structures in an easily understood manner.
- It is proved that under a constraint on the minimum correlation desired, there is a specific structure on the correlations between variables that allows edge relationships to be mapped to the vertices, and thus allows *complex sets* to capture the same information as *complete complex sub-graphs*.
- An algorithm is developed that mines all complex maximal sets of variables. This is a data mining technique, where the patterns mined highlight interesting and complex interactions between variables that would otherwise be hidden. Experiments show the algorithm is very efficient at mining such sets, due also in part to the extensive pruning it employs.

- The approach is further developed for mining a representative subset of the variables and in particular, for the feature subset selection problem. As a result, an unsupervised feature subset selection method is proposed. Experiments on the UCI cardiac arrhythmia data set show that it outperforms PCA when used for feature selection.

9.1.3 Organisation

The remainder of this chapter is organised as follows: Section 9.2 presents the theory, section 9.3 describes the data mining algorithm, section 9.5 describes the feature subset selection algorithm, section 9.6 provides experimental results, section 9.7 puts the contributions in the context of previous work, and section 9.8 concludes this chapter.

9.2 Complete, Complex Variable Sub-graphs, Sets and Correlation

Recall that the graph on the variables was defined as follows: each variable is a vertex and there is an edge between vertices if the corresponding variables are correlated: Given a threshold t, an edge exists between two variables A and B if $|\rho_{A,B}| \geq t$. The weight of the edge is $\rho_{A,B}$ and of specific interest is whether $\rho_{A,B}$ is positive or negative – called the *label* of the edge. Later, the problem of mining uncorrelated sets is also considered, where $|\rho_{A,B}| \leq t$.

Pearson's correlation coefficient between two random variables A and B is

$$\rho_{A,B} = \frac{cov(A,B)}{\sigma_A \sigma_B} = \frac{E((A-\mu_A)(B-\mu_B))}{\sigma_A \sigma_B}$$

If the data is centered, that is, $E(A) = E(B) = 0$, then

$$\rho_{A,B} = \frac{\vec{a} \cdot \vec{b}}{||\vec{a}||\,||\vec{b}||} = corr(\vec{a}, \vec{b})$$

where $\vec{a}$ and $\vec{b}$ are the vectors of samples for the variables A and B. In this work, $corr(\vec{a}, \vec{b})$ is used, and the data is assumed to be centered[1]. The use of the dot

[1] Centering the data is not necessary, and this is sometimes preferred in practice, but in that case it does not equal $\rho_{A,B}$.

product also means that the kernel trick is applicable – potentially allowing non-linear correlations to be used. However, this is not explored in this chapter.

Recall that the goal is to mine *complete*, *complex* and *maximal* sub-graphs of variables, and to be able to represent these as *complex maximal sets*. Recall that a sub-graph is *complete* if it is completely connected. A set will only ever be used to describe a *complete* sub-graph. Recall that the term *complex* describes the inclusion of negative and positive relationships (labellings of edges or variables). Recall that a complete sub-graph is called *maximal* if no other complete sub-graph subsumes it. Equivalently, a set is *maximal* if no super-set exists.

Section 9.2.1 considers the problem of mining maximal and complex sets of highly correlated variables – which is the focus of this paper. Section 9.2.2 briefly considers the problem of mining *uncorrelated* variables.

9.2.1 Highly Correlated, Complex Variable Sets

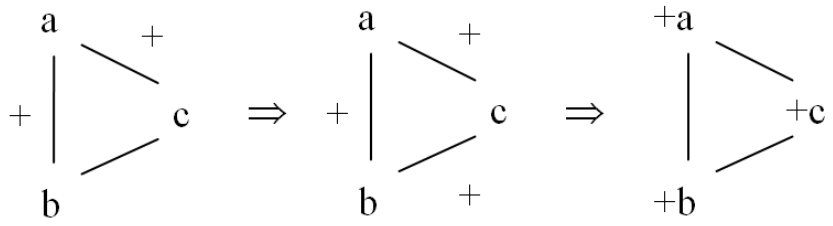
This section develops the theory required to mine highly correlated, complex variable sets.

Lemma 9.1. *$corr(\vec{a},\vec{b}) > t \wedge corr(\vec{b},\vec{c}) > t \wedge |corr(\vec{a},\vec{c})| > t \implies corr(\vec{a},\vec{c}) > t$ if and only if $t \geq 0.5$. In other words, if $(\vec{a},\vec{b})$ are highly positively correlated and $(\vec{b},\vec{c})$ are highly positively correlated and $(\vec{a},\vec{c})$ are highly positively or negatively correlated, then $(\vec{a},\vec{c})$ are in fact highly positively correlated. In this case, "highly" means with a correlation coefficient above 0.5.*

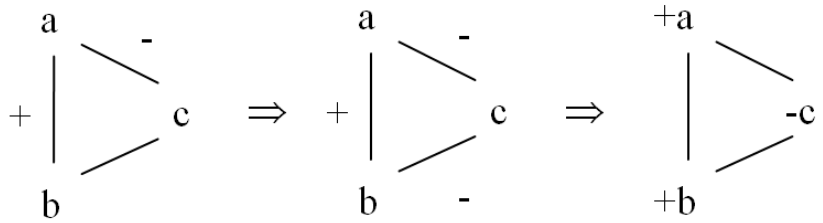
Proof. Without loss of generality, assume $\{\vec{a},\vec{b},\vec{c}\}$ are all unit vectors (this does not change the correlation: $\frac{\vec{a}\cdot\vec{b}}{||\vec{a}||\,||\vec{b}||} = (\frac{\vec{a}}{||\vec{a}||}\cdot\frac{\vec{b}}{||\vec{b}||})/(||\frac{\vec{a}}{||\vec{a}||}||\,||\frac{\vec{b}}{||\vec{b}||}||)$). Then $corr(\vec{a},\vec{b}) = \vec{a}\cdot\vec{b}$ – the dot product. The following identity is used: $\sum_i(a_i+c_i-b_i)^2 = \sum_i[(a_i^2+b_i^2+c_i^2)+2(a_ic_i-b_ic_i-a_ib_i)] = 3+2(\vec{a}\cdot\vec{c}-\vec{b}\cdot\vec{c}-\vec{a}\cdot\vec{b})$. The last equality follows as the vectors are unit vectors (i.e. $||\vec{a}|| = 1 \implies \sum_i a_i^2 = 1$). Using the thresholds $\vec{a}\cdot\vec{b} > t$ and $\vec{b}\cdot\vec{c} > t$ and the fact that $\sum_i(a_i+c_i-b_i)^2 \geq 0$ gives: $0 \leq 3+2(\vec{a}\cdot\vec{c}-\vec{b}\cdot\vec{c}-\vec{a}\cdot\vec{b}) < 3+2\vec{a}\cdot\vec{c}-4t$.

To avoid a contradiction we must therefore have $\vec{a}\cdot\vec{c} \geq 2t-1.5$ If $\vec{a}\cdot\vec{c} < -t$ then $-t > 2t-1.5 \iff t < 0.5$. Therefore, when $t \geq 0.5$, $a\cdot c < -t$ provides a contradiction and therefore we must have $\vec{a}\cdot\vec{c} > t$.

In the reverse direction, we have $\vec{a}\cdot\vec{c} > t$ (as the implication is true). Suppose for the purpose of a contradiction that $t < 0.5$. Then we can see from $\vec{a}\cdot\vec{c} \geq 2t-1.5$ that it is possible to have $\vec{a}\cdot\vec{c} < -t$ – providing the contradiction (for example substitute any value $t < 0.5$). □



(a) Lemma 9.1 followed by Theorem 9.3.



(b) Corollary 9.2 followed by theorem 9.3.

Figure 9.1: Simple Example of the lemma and corrolaries for sub-graphs of size 3. Recall that an edge exists between two variables a, b if $|corr(a, b)| \geq t$. It is assumed $t \geq 0.5$ so the lemma and corrolaries apply. In the first step (implication) in (a), lemma 9.1 is applied. In the first step in (b), corrolary 9.2 is applied. The second step of both (a) and (b) shows the application of corrolary 9.3, choosing a as the arbitrary + variable. Hence, the relationships can be represented as the complex sets $\{a, b, c\}$ for (a) and $\{a, b, -c\}$ for (b).

A corrolary follows immediately:

Corollary 9.2. *$corr(\vec{a}, \vec{b}) > t \wedge corr(\vec{b}, \vec{c}) < -t \wedge |corr(\vec{a}, \vec{c})| > t \implies corr(\vec{a}, \vec{c}) < -t$ if and only if $t \geq 0.5$*

Proof. Replace $\vec{c}$ with $-\vec{c}$ in lemma 9.1. □

These are illustrated graphically in the left hand implications of figures 9.1 (a) and (b).

These results imply that given a complete complex sub-graph of size three, the sign of the third edge can be obtained from the sign of the other two, simply by multiplying them together. Since this works for any triple in a complete sub-graph, this can be extended to the entire sub-graph. Furthermore, it allows the signs of the edges to be mapped to the variables themselves. The following corrolary describes this:

Theorem 9.3. *If $t \geq 0.5$, then relationships between variables in a complete sub-graph can be assigned to the variables themselves (without loss of information) using*

the following procedure:

1. *Select an arbitrary variable a and label it $+$.*
2. *For each other variable b in the sub-graph, label it according to the sign of it's correlation to a.*

All relationships between two variables can be inferred (reconstructed) from their labeled sign: if they have the same (different) sign, they have a positive (negative) correlation.

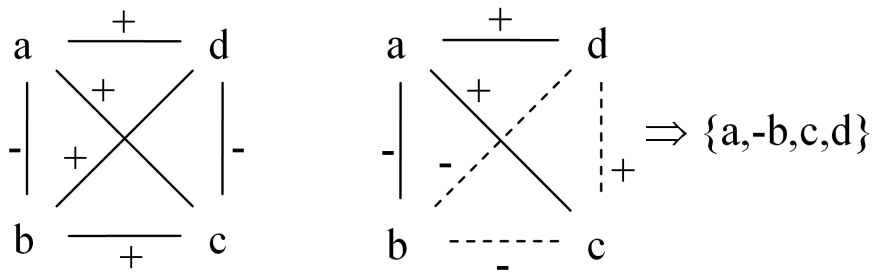
Proof. In the procedure, every variable $b \in V : b \neq a$ will clearly be assigned only one sign. It suffices to show that after this has been done, the reconstruction of edge signs works. Consider two variables $b \neq a$ and $c \neq a$. By the construction, the sign of their correlation with a is known. The sign of $corr(b, c)$ can therefore be determined by lemma 9.1. By considering all such pairs (b, c), every edge's sign can be constructed. □

Actually, there are exactly two ways of labeling every complete complex sub-graph, both of which express exactly the same edge relationships. In theorem 9.3, a may be arbitrarily labeled $-$ (instead of $+$), which simply flips all the other signs also. Of course this would be redundant, hence only one representation is used. In the algorithm, an arbitrary order is imposed on variables and the greatest variable in a sub-graph is arbitrarily chosen to be $+$. A simple example is shown in figure 9.1.

Theorem 9.3 also means that the sign of the edges between variables in the graph can be assigned to the variables themselves. This has two important consequences:

- *Complex sets* completely describe the relationships. This means that with the assigned signs, every variable in a complex set is highly positively correlated with each other variable in the set. This makes the structure very easy for the user to understand as a set is a simpler construct than a graph.
- The search space of the mining algorithm is significantly decreased, as the problem is reduced to mining sets of variables, rather than sub-graphs.

Observe that the inclusion of negative correlations only makes sense if theorem 9.3 holds – otherwise it is not possible to assign the direction of the correlation *between* variables to the variables themselves: When $t < 0.5$ it is not possible to report a set of variables such as $\{a, -b, c, d\}$ with the interpretation that these four variables are



(a) A configuration like this is possible only when $t < 0.5$. It cannot be mapped to a complex set.

(b) When $t \geq 0.5$, any complete complex sub-graph can be mapped to a complex set. The signs on the dotted edges can be inferred from the others.

Figure 9.2: Example of corrolary 9.3

highly positively correlated with each other, since it is possible that $corr(a, b) < -t$, $corr(a, c) > t$ but $corr(b, c) > t$. In this case there exists no labeling of variables that can produce a set so that each element is positively correlated with the others. Accordingly, complex sets are not meaningful when $t < 0.5$. The reader may like to try this on the example in figure 9.2(a). Following the procedure of theorem 9.3 does not work as the edges cannot be reconstructed, so it is impossible to map the complex sub-graph it to a complex set. On the other hand, the example in figure 9.2(b) does work and demonstrates the procedure.

In section 9.3, a method of enumerating the possible sets will be presented that, in conjunction with theorem 9.3, means that all complex complete variable sets can be mined and labeled in $O(2^{|V|})$ time – the same complexity as without considering the sign of the correlations. For comparison, note that a naive approach would be to enumerate possible sets, and for each, apply corrolary 9.3. This would require $O(|V| \cdot 2^{|V|})$ time due to the $O(|V|)$ operations used for labeling the extra $O(|V|)$ edges added whenever another variable is added in the search.

9.2.2 Uncorrelated Variable Sets

An interesting but simpler problem is to find maximal sets of variables that are pairwise uncorrelated, in the sense that the absolute correlation is below a threshold. That is, an edge exists between two variables A and B if $|corr(A, B)| \leq t$, where t is a (usually small) threshold. This mines sets of uncorrelated variables. Of course, complex relationships don't make sense for these.

9.3 Mining Complex Maximal Sets: Algorithm

9.3.1 Algorithm

Recall from section 3.3.1 that a $PrefixTree$ can be used to represent the search space for mining interactions. Here, each node in the prefix tree (called a $Node$ in algorithm 9.1) corresponds to a complete set of variables. Without loss of generality, assume the variables are integers $V = \{1, 2, ..., n\}$. The only information stored at each node is a variable (v) and a sign label ($sign$). For ease of presentation, consideration of the sign is deferred for the moment.

The algorithm (algorithm 9.1) works by performing a depth first traversal of the search space, expanding sibling nodes in *increasing* order – which is important as described later – and pruning the search as soon as possible.

Specifically, the following properties are exploited. Here, a set is called complete if the corresponding sub-graph is complete. Elsewhere in the paper this is implicit.

1. Whenever a new variable v_2 is considered to be added to a complete set C, and v_2 is not highly correlated with *each* variable in C, then neither $C \cup v_2$ or any super-set of $C \cup v_2$ can be complete. That is, the corresponding sub-graphs will also be missing at least one edge. *One* consequence of this is the following: Since by construction $v_2 < v_1 \forall v_1 \in C$, the entire sub-tree rooted at the node corresponding to $C \cup v_2$ may be pruned. The case $C = \emptyset$ holds trivially by defining it as complete.

2. When checking whether a new variable v_2 can be added to a complete set $C \cup v_1$, the algorithm only needs to consider those v_2 for which $C \cup v_2$ is complete, by property 1. That is, if $C \cup v_2$ is not complete, then neither can its super-set $C \cup v_1 \cup v_2$ be. Now, if $C \cup v_1$ and $C \cup v_2$ are complete, then $C \cup v_1 \cup v_2$ is complete if and only if $v_1 \cup v_2$ is complete (that is, if and only if v_1 and v_2 are highly positively or negatively correlated). The reason for this is straightforward: the only edge that can be missing in the sub-graph defined by $C \cup v_1 \cup v_2$ is (v_1, v_2), as the existence of all the other edges has already been established. Translated to the prefix tree and the algorithm, this means that only *siblings* need to be considered – note that $C \cup v_1$ and $C \cup v_2$ will become siblings in the prefix tree, with common prefix C. The algorithm is said to progress by *joining siblings*.

3. The above two properties also work in combination. If $C \cup v_2$ is not complete, then neither can $C \cup v_1 \cup v_2$ be. By never creating the node for $C \cup v_2$ (recall

this part of the search space is pruned), $C \cup v_1$ will have one less sibling that must be considered.

In algorithm 9.1, properties 2 and 3 are achieved using the *newSiblings* list, which is used as the *siblings* list for expanding new child nodes in the depth first search. Property 1 is achieved by not adding the corresponding node or expanding the search (no recursive call). Note that the for loop in algorithm 9.1 traverses the siblings in increasing order.

It can be of use to report the minimum correlation between any pair or variables in a set. This is useful, as it provides a bound that is generally higher than t. This can be achieved by storing the minimum at the corresponding node, and computing the new minimum for a new node as the minimum over the siblings and the additional link.

Note that the algorithm works by growing sets, and using heavy pruning. This approach is appropriate when the graph of correlations is sparse – precisely what happens when high correlations are desired.

9.3.2 Complex Sets

The only thing left in the search part of the algorithm is to label the variables. Accordingly, recall that each node also has a sign associated with it – either + or − (in the algorithm, $Node.sign$). The sign corresponds to the relationship that the node's variable has to the *first* node in the sequence – the node whose parent is the root.

Without loss of generality[2], the children of the root are labeled +. The sign of a new node is calculated as follows. When joining the siblings corresponding to $C \cup v_1$ and $C \cup v_2$, the sign of $C \cup v_1 \cup v_2$ is the sign of $C \cup v_1$ multiplied by the sign of the correlation between v_1 and v_2. This is a direct consequence of lemma 9.1 and corrolary 9.2 applied to the variables v_1, v_2 and x, where x is the *first* node in the sequence (the first element of C). Note that this is the application of the procedure in theorem 9.3. Furthermore, by that theorem, the signs of the relationships between any of the variables can be derived from the sign of the node (variable). When the sets are output by a traversal toward the root, the sign also becomes the sign of the variable.

[2]There are two equivalent labellings for variables in complex sets – just flip the sign of each variable.

9.3.3 Maximal Complex Sets

The algorithm must also calculate the *maximal* complex sets. It does this by maintaining the current maximal sets, and as new sets are added, deleting any subsets. Labels can be ignored during this process. The following lemma makes this easier.

Lemma 9.4. *Subsets of a set represented by a node currently being examined can only occur in a part of the tree that has already been examined by the algorithm.*

Proof. This can be proved analogously to lemma 3.18. □

Note that this is why the order of expansion of siblings is important. More specifically, maintaining a consistent (but possibly arbitrary) order is important.

The algorithm only updates the *maximalSets* list with sets (nodes) that are known to be maximal *so far* and *in the near future* in the search. The first constraint is trivially met by lemma 9.4. The second constraint is met by adding those sets (nodes) that have no children when that path is complete, as such a set may only be a subset of a node on a different path of the search, which occurs later (that is, only after the current path is completed). Because of lemma 9.4, new maximal sets can only replace existing ones, and therefore only sets that have been mined earlier must be checked for being subsets of a new one.

Finally, note that since the *Prefix-Tree* shares as many nodes as possible, the space of the collection of maximal sets is minimized since prefixes of the stored maximal sets are shared.

Considering all of the above, the resulting algorithm can be written surprisingly simply – especially in recursive form as shown in algorithm 9.1.

9.3.4 Mining Uncorrelated Sets

In order to mine sets where each variable is uncorrelated with every other, algorithm 9.1 is modified as follows. "$|corr(v_1, v_2)| \geq t$" in $mine(\,,\,,\,)$ is replaced with "$|corr(v_1, v_2)| \leq t$", and "return 1" in $corr(\,,\,)$ is replaced with "return 0". The *sign* of the variables should also be ignored, as they cannot represent all relationships.

However, it should be pointed out that data sets generally have many uncorrelated variables, so using the enumeration approach of algorithm 9.1 is not the most practical method as it is designed for mining sets defined by high correlations, as this allows it to take maximum advantage of the pruning abilities.

Algorithm 9.1 Simplified algorithm for mining complete and maximal complex correlated sets when $t \geq 0.5$. The algorithm assumes a garbage collector, or an alternative approach to delete nodes in the *Prefix-Tree* that are no longer required.

Input:
double corr[][] //precomputed correlation matrix
double t //correlation threshold, $t \in [0,1]$
Output:
maximalSets //complete, maximal sets
//as PrefixTree nodes
Data Type:
Node(Node parent, int v, int sign)
//nodes in the PrefixTree

$List\langle int\rangle\, V = [1,2,...,corr[0].length]$ *//variables*
$List\langle Node\rangle\, maximalSets = \emptyset$
$mine(V, \emptyset, Node(null, \infty, 1))$ *//*

$mine(List\langle int\rangle\, siblings, List\langle int\rangle\, newsiblings, Node\, n)$
$int\, v_1 = n.v$
$boolean\, hasChild = false$
for each ($int\, v_2$ in $siblings$)
if ($|corr(v_1, v_2)| \geq t$)
$Node\, nn = Node(n, v_2, n.sign * corr(v_1, v_2))$
$mine(newsiblings, \emptyset, nn)$ *//recursive, DFS*
$newsiblings.add(v_2)$ *//new sibling was created*
$hasChild = true$
else *//no need to expand search*
if (!$hasChild$) *//super-set known to exist*
$addCompleteSet(n)$ *//n is maximal so far*

$addCompleteSet(Node\, n)$
for each ($Node\, n_2$ in $maximalSets$)
if (n_2 subsetof n) *//simple linear traversal*
$maximalSets.remove(n_2)$ *//not maximal*
$maximalSets.add(n)$

$double\, corr(int\, v_1, int\, v_2)$
if ($v_1 = \infty$) return 1 *//root of PrefixTree.*
else return $corr[v_1 - 1][v_2 - 1]$

9.3.5 Complexity

For completeness, this section briefly considers the worst case complexity of the algorithm and can be skipped without loosing the flow of the chapter.

Lemma 9.5. *The time complexity of algorithm 9.1 is at most* $O(|V|^2 \cdot |S|) + O(2^{|V|}) + O(|V| \cdot 2^{2|V|}) = O(|V| \cdot 2^{2|V|})$*, where* $|S|$ *is the number of samples.*

Proof. Calculating the correlations is done in $O(|V|^2 \cdot |S|)$, enumerating the sets takes at worst $O(2^{|V|})$ (the number of nodes in the search), since there are a constant number of operations per node (recall this is a consequence of exploiting the theory in this chapter). The maximum number of maximal sets is bounded above by $2^{|V|}$, and computing the maximal sets given m candidates takes $m^2/2$ comparisons, each of which is $O(|V|)$ (traversal of the node sequence to check whether one is a subset). Hence this part is $O(|V| \cdot 2^{2|V|})$. □

In practice, due to the nature of real data sets and the pruning used, this is not a realistic reflection of run time performance. In particular, the computation of maximal sets generally takes *less* time that the enumeration of sets, despite having higher worst case complexity. This is because the set of maximal sets is continually reduced as the algorithm progresses (which is not reflected in the worst case), and the number of candidate maximal sets is much fewer that the number of sets enumerated by the search. Finally, the worst case occurs when every variable is highly correlated with every other variable, which generally does not happen in practice.

Lemma 9.6. *The space complexity is at most* $O(|V|^2) + O(|V|^2) + O(\begin{pmatrix} |V| \\ |V|/2 \end{pmatrix}) < O(2^{|V|})$

Proof. This is simply the space of the correlation matrix, plus the space of a depth first search including the sibling list (the maximum depth and sibling list size is $|V|$), plus the maximum number of maximal item-sets at any one time. It can be shown that the latter is $\begin{pmatrix} |V| \\ |V|/2 \end{pmatrix}$, since this is the maximum number of subsets of equal size, and the maximum number of maximal sets must all have equal size (proof omitted). A bound on this is $2^{|V|}$. □

Again, in practice this is misleading since computing the maximal sets continuously

prunes the list. If needed, an alternative disk based method for processing the maximal sets can easily reduce the memory requirement.

9.4 Mining the Patterns using GIM

The reader may have noticed that the preceding algorithm has some similarities to the GIM algorithm. GIM is an abstract approach and generalisation developed by considering many different problems and drawing inspiration from solving them efficiently. The problem in this chapter is one of these. Accordingly, with a small modification, GIM can be used to solve this problem too. Showing how to mine cliques and maximal cliques with GIM was covered in section 3.8. However, this does not include the ability to handle positive and negative patterns, or the labeling of the nodes. Using the method for handling negative variables outlined in section 3.6 is inefficient for the problem in this chapter, since it was proved that the correlation structure is such that only certain structures are possible. Hence, to implement the approach in GIM, one can start with the method described in section 3.8 as the basis, and cleverly implement the labeling within the $M_I(\cdot)$ function. Note from algorithm 9.1 that the labeling of a new node nn requires access only to the current node n to obtain its *sign*, and the sign of the correlation between $n.v$ and the variable v_2. Hence, to compute the sign of nn, $nn.parent.sign$ is multiplied with the sign of the correlation between $nn.v$ and $nn.parent.v$. This can be done as follows:

$\texttt{evaluate}M_I(PrefixNode\, nn)$
  $PrefixNode\, n = nn.parent;$
  $return\ \ [n.value_M[0] * corr(nn.variableId, n.variableId)]$

Where $nn.value_M$ is an array of size one and $value_M[0]$ is equivalent to the *sign* in algorithm 9.1. Since $M_I(\cdot)$ only requires access to the current node and its parent, which can be reached directly through the *parent* link, there is no need to store any prefix nodes. Accordingly, `store(·)` does nothing and the prefix tree is not retained in memory.

9.5 Selecting a Representative Set: an Application to Feature Subset Selection

Recall that maximal sets of correlated variables can be presumed to capture sets of variables that are interchangeable with each other and therefore can be represented

by one member of the set. In this section, this idea is developed for the purpose of feature subset selection. The goal is to select variables in such a way that they "cover" (represent) the original data set, but at the same time are not correlated with each other. The primary complication is the overlap between maximal sets of variables, which requires some care. The approach is as follows:

1. Mine all maximal sets, where variables are connected if $|corr(A, B)| \geq t$, using algorithm 9.1. Call the result – a set of such sets – M. Note that a set containing a single variable may be maximal. Clearly, all variables will be present in at least one element of M and in that sense, the data set is completely "covered".

2. Select a representative variable from each maximal set $C \in M$. This is a two step procedure, complicated by overlap between elements of M:

   (a) Recall that the weight of each edge (v_i, v_j) is the correlation between the variables. For each $C \in M$ select the representative variable $v \in C$ as follows, breaking ties arbitrarily:

   $$v = \arg\max_{v}(\sum_{v_j \in C} |corr(v, v_j)|)$$

   In other words, the most central variable is chosen, measured by it being the most correlated with all the other variables in the set C. The variable v is taken to represent the other variables and to capture the underlying factor of the set. The remaining variables $C - \{v\}$ are assumed to be redundant.

   (b) Due to the frequent overlap between the $C \in M$ (different maximal sets often share a common subset), it is not possible to treat each C in isolation, as a redundant variable in one maximal set may be the representative (non-redundant) variable of another – overlapping – maximal set. The problem with this is that two or more variables can be chosen that are in fact in the same maximal set (and therefore correlated with each other). To partially remedy this, assign each variable $v \in V$ an integer weight. When considering each $C \in M$ as above, the chosen variable $v \in C$ has it's weight incremented by the number of variables it replaces in C – that is, $|C|$. Every other (redundant) variable $v' \in C - \{v\}$ has it's weight decremented by $|C| - 1$. Note that a variable may be determined to be a representative (redundant) variable for some $C \in M$, but a redundant (representative) variable in other C('s).

Only variables with a positive weight after the procedure has completed are retained. This means that a variable is only retained if it is more representative than non-representative, measured by the number of variables it represents minus the number of variables that it does not represent. The reason for decrementing by $|C| - 1$ rather than C is to avoid variables "canceling" each other out when representing two overlapping sets of equal size.

Call the resulting set of variables V_c. Generally, V_c contains fewer variables than V and so the number of features has been reduced. However, V_c is only considered a candidate set of selected features, as it's elements may still be correlated with each other. This can occur, for example, when two sets of equal size overlap, or when two sets are connected to each other. In the latter case they don't overlap, but some elements of one set may be correlated with elements of the other. This is undesirable, as the selected variables should not be correlated with each other.

3. This step ensures that none of the selected variables are correlated with each other. First, the "cumulative sum" of correlations is computed for each variable:

$$cum\_sum(v) = \sum_{C \in M} \sum_{v_j \in C, v \neq v_j} |corr(v, v_j)|$$

Note that this can be done as part of step 2a. A variable with a higher cumulative sum is more representative, and therefore is more desirable. This is used to decide between pairs of correlated variables. The procedure is as follows;

Loop through each $v \in V_c$, and check if it is correlated with another variable $v' \in V_c$. If not, add v to V_s. If it is, add it to V_c' *if* the cumulative sum of it's correlations (as described above) is higher than that of v'. Set V_c to V_c' and repeat the procedure until V_c is empty. The final set of selected variables is V_s.

Note that complex relationships are not applicable for feature selection. That is, of interest is only whether there is a high correlation – the sign of the correlation is irrelevant. Therefore, algorithm 9.1 can be used as Step 1 of the feature selection procedure for any value of t.

Note that this is an unsupervised approach. If a variable to be predicted is present, it must be removed from $|V|$ prior to applying the procedure.

The approach "covers" the data set, in the sense that every variable is taken into account by the final selected set – provided that this does not lead to selected attributes being correlated with each other.

Data set	Attributes	Instances
MADOLEN	500	2000
SYLVA	216	13086
Arrhythmia	279	452

Figure 9.3: Data set properties.

The threshold t functions in two ways: First, it allows the user to define the minimum correlation magnitude between variables that signifies that variables can be considered redundant. Secondly, no variables in the final selected set will be correlated with each other (have a correlation magnitude greater than t). The technique therefore generates a *representative* subset of the original variables while guaranteeing that the selected variables are uncorrelated.

An advantage of this feature selection approach, in addition to the guarantees provided on the correlations and redundant features, is the simplicity of the resulting features – they are just variables.

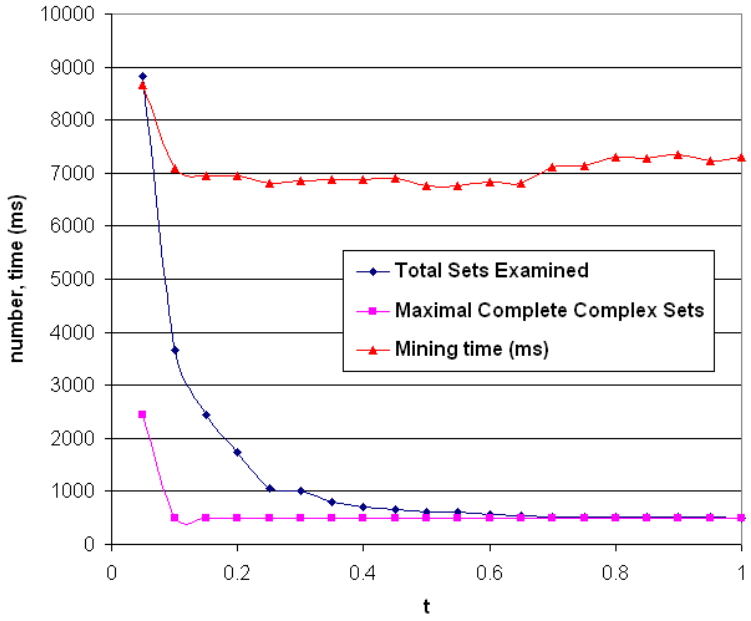
9.6 Experiments

An implementation of algorithm 9.1 is first evaluated on some large data sets for the purpose of run time analysis. Then, the approach is applied to feature selection using the technique described in section 9.5.

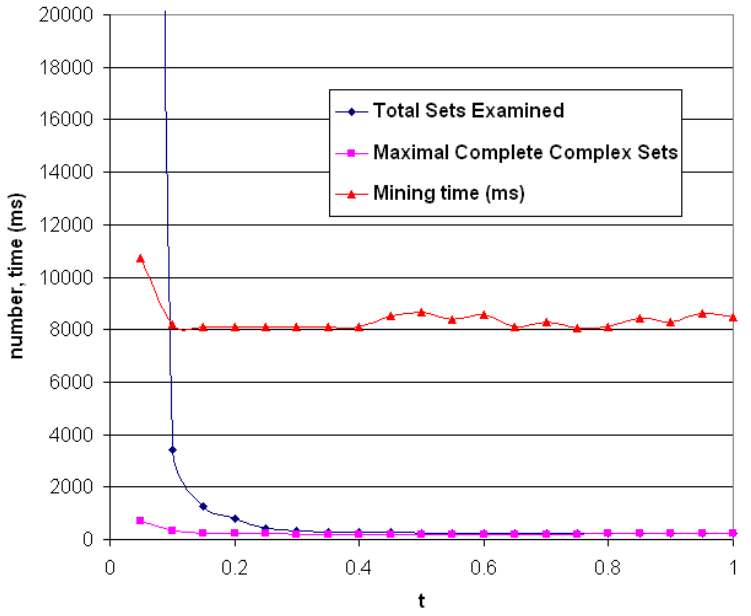
9.6.1 Run Time Performance

Experiments were performed on three data sets: MADOLEN, SYLVA and Arrhythmia. The MADOLEN data set was obtained form [67] and SYLVA was obtained from [102]. The data sets were part of feature selection and performance prediction challenges respectively. No pre-processing was done on them and the "training data" sets were used. The Arrhythmia data set was obtained from the UCI repository [2], and all missing values replaced by the mean of the corresponding attribute. In all data sets, the class variable was omitted. All data sets were chosen for a large number of numeric features and high density in order to attempt to challenge the algorithm. In particular, the Arrhythmia data set is one of the larger data sets in the UCI repository, and due to the problem domain, many variables are related. Properties of the data sets are listed in figure 9.3.

The run time results for various levels of t are shown in figures 9.4 and 9.5. For the SYLVA and MADELON data sets (figure 9.4) the run time remains relatively

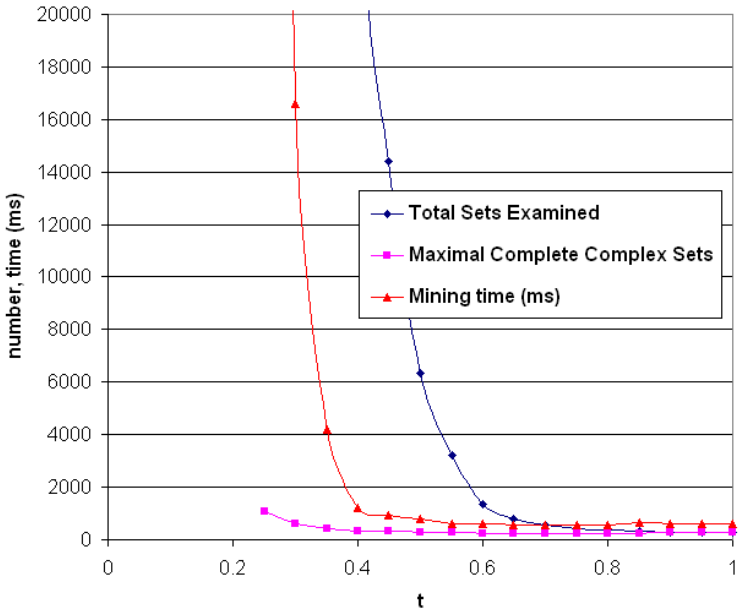


(a) MADELON Dataset

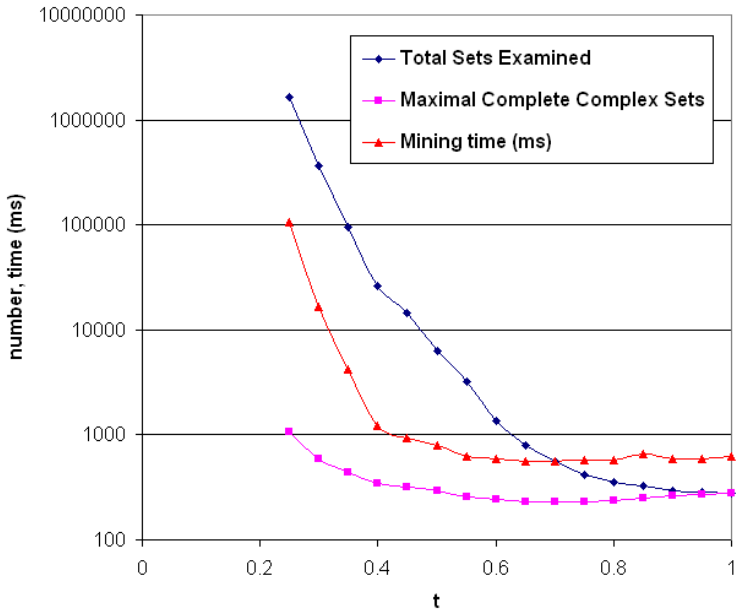


(b) SYLVA dataset

Figure 9.4: Run time results part 1. See also figure 9.5. Total Sets Examined is the exact number of sets that the search has examined. That is, the size of the space examined. Maximal Complete Complex Sets is the number of such sets mined. Mining time is the run time of the entire algorithm in milliseconds.



(a) Arrhythmia Dataset



(b) Arrhythmia Dataset, vertical axis in log scale

Figure 9.5: Run time results part 2. See also figure 9.4.

Algorithm	Accuracy, original data set	Accuracy, after PCA	Accuracy, reduced data set	Accuracy improvement over original data set	Accuracy improvement over using PCA
J48	76.99	66.81	65.04	-11.95	-1.77
J48graft	78.32	67.48	65.71	-12.61	-1.77
NaiveBayes	76.99	71.68	72.12	-4.87	0.44
IBK, K=5	63.72	57.74	63.94	0.22	6.19
IBK, K=1	63.72	57.30	62.39	-1.33	5.09
DecisionStump	65.93	60.62	64.60	-1.33	3.98
ZeroR	54.20	54.20	54.20	0.00	0.00
OneR	54.20	59.07	54.87	0.66	-4.20
DecisionTable	71.68	68.14	66.37	-5.31	-1.77
ADtree	79.65	71.02	67.92	-11.73	-3.10
BaysianNet	77.21	72.12	70.35	-6.86	-1.77
Jrip	65.27	61.50	65.93	0.66	4.42
SimpleCart	77.88	68.36	69.03	-8.85	0.66
RandomForest	75.00	66.81	69.25	-5.75	2.43
Kstar	57.52	53.98	63.05	5.53	9.07
Logistic	63.27	67.48	69.47	6.19	1.99
SimpleLogistic	75.22	74.78	71.68	-3.54	-3.10
PART	76.77	72.12	68.81	-7.96	-3.32
Average	69.64	65.07	65.82	-3.82	0.75

Figure 9.6: Accuracy results for various Classifiers on the Arrhythmia data set.

constant. It is only when the threshold becomes very small that the search space expands significantly. In the Arrhythmia data set (figure 9.5) on the other hand, many more correlations are exhibited. Indeed, this is expected as the variables in the data set are related in the domain. A threshold of $t = 0.2$ took over 10 minutes, at which point the experiment was stopped.

The results also show that on these data sets, which are presumed to be typical, there are relatively few complete maximal sets when t is above about 0.4. This means that the enumeration approach considered is ideal, as it allows heavy pruning of the search space and therefore allows it to progress quickly.

9.6.2 Feature Selection Performance

The approach of section 9.5 is used here to perform feature selection on the Arrhythmia data set. t was set to 0.5, resulting in 111 attributes being selected out of the 279 original attributes. If only positive correlations are considered, 135 attributes would have been selected.

In addition to comparing classification results on the reduced data set to the original data set, a comparison to PCA was also performed. PCA was performed using the algorithm from WEKA [104], and options were set so the same number of attributes – 111 – were chosen. The 111 principle components cover 96% of the variance of the data set.

Figure 9.6 shows the results on various classifiers in WEKA [104] (version 3.5.7), evaluated over the original data set, the data set with features extracted using PCA, and the subset of the attributes selected using the approach in section 9.5. Unless otherwise stated, default values were used in the ML algorithms. The 16 classes in the original data set were amalgamated into two classes, representing normal heart rhythms (245 instances) and cardiac arrhythmia (207 instances). 10-fold cross validation was used for the evaluation of classification accuracy in all cases. The approach in this paper performs comparably to PCA, having only 0.75 percentage points better accuracy on average. On average, the accuracy is 3.82% lower than on the original data set. Therefore, not only can this approach compete well against PCA, but it maintains the interpretability of the model. That is, the rules and decision trees built on the data set retain the actual attributes, in contrast to when PCA is used.

9.7 Related Work

9.7.1 Clique and Set Mining

A complete set and a clique are equivalent. The latter is often used in social network situations or in spatial data sets. In spatial applications, the space in which variables exist is usually low dimensional so enumeration approaches to mine them are not appropriate. Also, distances are used, rather than correlations (angles). “Complex” cliques have been considered [64], but this is in relation to *absence* of objects.

Graph based clustering approaches are also related. In some sense, the approach described in this paper is related to agglomerative clustering [88]. The desire for complete sub-graphs (sets) is the same as the clique pattern, or in distance based approaches, the MAX approach [88]. The maximal set idea could be considered as the highest level in a hierarchy defined over subsets, but the method does not fit into hierarchical clustering. In particular, the threshold is fixed. The approach in this paper is not really a clustering method. It is best described as a method of mining interactions between variables, with those interactions having a specific structure and being defined by correlation. The consideration of complex interactions in particular

sets it well apart from clustering approaches.

The algorithmic approach has a closer relationship to itemset mining than it does to clustering. Items are a special type of variable, and itemsets are sets of variables possessing some interesting property – usually that they occur frequently. The similarity to item enumeration approaches is that the enumeration is over sets of variables, from the bottom up. The fundamental difference to itemset mining is that the itemset mining problem cannot be mapped to graph mining, as it cannot be reduced to pairwise relationships. Complex relationships therefore also don't mean the same thing. While the *absence* of an item can be considered, this is different to the complex relationships (both negative and positive correlations) considered in this chapter.

It should also be emphasised that the use of correlation is a core component of this work, in particular, the lemma and corollaries that are developed under the completely connected sub-graph structure. Correlation is generally not used for clustering, and it cannot be used for itemset mining, as it does not translate to more than two variables at a time. Unlike distance measures, it has both positive and negative values – therefore techniques based on it necessarily have different semantics.

9.7.2 Feature Subset Selection

Feature subset selection comes in three flavours; wrapper, embedded or filter [88]. In the wrapper or embedded approaches, it is used in conjunction with a data mining or machine learning algorithm in some form of supervised or semi-supervised process. The wrapper approach uses the DM or ML algorithm as an objective function, while in the embedded approach the DM or ML algorithm decides what features to discard as part of its operation. The filter approach selects a subset independently of the subsequent DM/ML algorithm. It may or may not be supervised. The approach described in section 9.5 fits into the unsupervised filter category. One filter approach using correlation for feature subset selection is presented in [45]. However, this is a hill climbing, supervised, optimizing approach. It is also based on entropy – not statistical correlation.

Finding representative sets is considered in [70] using an entropy based approach on binary data. The algorithm in [70] also mines a representative set directly (this work performs it as a second step).

As earlier mentioned, the idea of maximal complex sets representing underlying factors of the data set has similarities to the way principle components can be applied.

But as also mentioned earlier, these are very different approaches.

In summary, the work in this paper is related to various bodies of work in Data Mining, but to the author's knowledge, is quite different to each.

9.8 Conclusion

This chapter presented and exploited useful results about the correlation structures between variables. Additionally, it proposed the 'complete, complex and maximal sub-graphs or sets of highly correlated variables' pattern. This approach is useful as a data mining technique in its own right, or, as also demonstrated in this paper, as the core component of an unsupervised feature subset selection procedure.

Solving the problem considered in this chapter was one of the many inspirations behind developing the generalised interaction mining approach introduced in this thesis.

A useful avenue of future work is to consider only significant patterns. For example, considering correlation graphs defined by significant correlation, in order to reduce the effects of noise and the probability that seemingly interesting patterns are found by chance alone.

Part IV

Mining Uncertain and Probabilistic Databases

Chapter 10

Probabilistic Frequent Itemset Mining in Uncertain Databases

Probabilistic frequent itemset mining in uncertain transaction databases semantically and computationally differs from traditional frequent itemset mining techniques applied to standard "certain" transaction databases. The consideration of existential uncertainty of item(sets), indicating the probability that an item(set) occurs in a transaction, makes traditional techniques inapplicable. This chapter introduces new probabilistic formulations of frequent itemsets based on possible world semantics. In this probabilistic context, an itemset X is called frequent if the *probability* that X occurs in at least *minSup* transactions is above a given threshold τ. This is the first approach addressing this problem and does so under possible worlds semantics. In consideration of the probabilistic formulations, a framework is presented which is able to solve the Probabilistic Frequent Itemset Mining (PFIM) problem efficiently. An extensive experimental evaluation investigates the impact of the proposed techniques and shows that the approach is orders of magnitude faster than straight-forward approaches.

10.1 Introduction

Association rule analysis is one of the most important fields in data mining. It is commonly applied to market-basket databases for analysis of consumer purchasing behaviour. Such databases consist of a set of transactions, each containing the items a customer purchased. The database can be analyzed to discover associations among different sets of items. The most important and computationally intensive step in the mining process is the extraction of *frequent itemsets* – sets of items that occur in at least *minSup* transactions.

It is generally assumed that the items occurring in a transaction are known for certain. However, this is not always the case. For instance;

- In many applications the data is inherently noisy, such as data collected by sensors or in satellite images.
- In privacy protection applications, artificial noise can be added deliberately in order to prevent reverse engineering of the data through pattern analysis [107]. Finding patterns despite this noise is a challenging problem.
- Data sets may also be aggregated. By aggregating transactions by customer, it is possible to mine patterns across customers instead of transactions. In the resulting database, this produces estimated purchase probabilities per item per customer rather than certain items per transaction. This application is used as an example later.

In such applications, the information captured in transactions is *uncertain* since the existence of an item is associated with a likelihood measure or existential probability. Given an uncertain transaction database, it is not obvious how to identify whether an item or itemset is frequent because we generally cannot say for certain whether an itemset appears in a transaction. In a traditional (certain) transaction database, one can simply perform a database scan and count the transactions that include the itemset. This does not work in an uncertain transaction database.

Dealing with such databases is a difficult but interesting problem. While a naive approach might transform uncertain items into certain ones by thresholding the probabilities [1], this loses useful information and leads to inaccuracies. Existing approaches in the literature are based on expected support, first introduced in [26]. Chui et. al. [25, 26] take the uncertainty of items into account by computing the

[1] For example, by treating all uncertain items with a probability value higher than 0.5 as being present, and all others as being absent.

expected support of itemsets. Itemsets are considered frequent if the expected support exceeds *minSup*. Effectively, this approach returns an estimate of whether an object is frequent or not with no indication of how good this estimate is. Since uncertain transaction databases yield uncertainty with respect to the support of an itemset, the probability distribution of the support and, thus, information about the confidence of the support of an itemset is very important. This information, while present in the database, is lost using the expected support approach.

Example 10.1. Consider a department store selling various types of products. To maximize sales, customers may be analysed to find sets of items that are all purchased by a large group of customers. This information could be used for advertising directed at this group. For example, by providing special offers that include all of these items along with new products, the store can encourage new purchases. Figure 10.1(a) shows such customer information. Here, customer A purchases games every time he visits the store and music (CDs) 20% of the time. Customer B buys music in 70% of her visits and videos (DVDs) in 40% of them. The supermarket uses a database that represents each customer as a single *uncertain transaction*, shown in figure 10.1(b).

10.1.1 Uncertain Data Model

The uncertain data model applied in this paper is based on the possible worlds semantic with existential *uncertain items*.

Definition 10.2. An *uncertain item* is an item $x \in I$ whose presence in a transaction $t \in T$ is defined by an *existential probability* $P(x \in t) \in (0, 1)$. A *certain item* is an item where $P(x \in t) \in \{0, 1\}$. I is the set of all possible items.

Definition 10.3. An *uncertain transaction* t is a transaction that contains uncertain items. A transaction database $T = \{t_1, \ldots, t_{|T|}\}$ containing uncertain transactions is called an *Uncertain Transaction Database* (UTB).

An uncertain transaction t is represented in an uncertain transaction database by the items $x \in I$ associated with an existential probability value[2] $P(x \in t) \in (0, 1]$. Example uncertain transaction databases are depicted in figures 10.1 and 10.2.

[2]If an item x has an existential probability of zero, it does not need to be recorded in the transaction.

Customer	Item	Probability item is purchased by customer
A	Game	1.0
A	Music	0.2
B	Video	0.4
B	Music	0.7

(a) Customer purchase probabilities.

Transaction Identifier	Transaction
t_A	$\{Game : 1.0, Music : 0.2\}$
t_B	$\{Video : 0.4,\ Music : 0.7\}$

(b) Corresponding uncertain transaction database.

World	Transaction database in world w_i	Probability world w_i exists ($P(w_i)$)
w_1	$t_A = \{Game\}$ $t_B = \{\}$	0.144
w_2	$t_A = \{Game, Music\}$ $t_B = \{\}$	0.036
w_3	$t_A = \{Game\}$ $t_B = \{Video\}$	0.096
w_4	$t_A = \{Game, Music\}$ $t_B = \{Video\}$	0.024
w_5	$t_A = \{Game\}$ $t_B = \{Music\}$ $t_A = \{Game\}$	0.336
w_6	$t_A = \{Game, Music\}$ $t_B = \{Music\}$	0.084
w_7	$t_A = \{Game\}$ $t_B = \{Video, Music\}$	0.224
w_8	$t_A = \{Game, Music\}$ $t_B = \{Video, Music\}$	0.056

(c) All corresponding possible worlds.

Figure 10.1: Example of a small uncertain transaction database and the possible worlds it generates.

Id	Transaction
t_1	$\{A : 0.8, B : 0.2, D : 0.5, F : 1.0\}$
t_2	$\{B : 0.1, C : 0.7, D : 1.0, E : 1.0, G : 0.1\}$
t_3	$\{A : 0.5, D : 0.2, F : 0.5, G : 1.0\}$
t_4	$\{D : 0.8, E : 0.2, G : 0.9\}$
t_5	$\{C : 1.0, D : 0.5, F : 0.8, G : 1.0\}$
t_6	$\{A : 1.0, B : 0.2, C : 0.1\}$

Figure 10.2: Example of a larger uncertain transaction database containing 6 transactions and items $\{A, B, C, D, E, F, G\}$. $A : 0.8$ states that the transaction contains item A with probability 0.8.

To interpret an uncertain transaction database, this chapter applies the *possible world model*: An uncertain transaction database generates *possible worlds*, where each world is defined by a fixed set of (certain) transactions. That is, each possible world corresponds to one certain transaction database. A possible world is instantiated by generating each transaction $t_i \in T$ according to the occurrence probabilities $P(x \in t_i)$. Consequently, each probability $0 < P(x \in t_i) < 1$ derives two possible worlds *per transaction*: One possible world in which x exists in t_i, and one possible world where x does not exist in t_i. Thus, the number of possible worlds of a database increases exponentially in both the number of transactions and the number of uncertain items contained in it.

Each possible world w is associated with a probability that that world exists, $P(w)$. Figure 10.1(c) shows all possible worlds derived from figure 10.1(b). For example, in world 6 both customers bought music, customer B decided against a new video and customer A bought a new game.

This work assumes that uncertain transactions are mutually independent. Thus, the decision by customer A has no influence on customer B. This assumption is reasonable in real world applications. Additionally, independence between items is often assumed in the literature [25, 26]. This can be justified by the assumption that the items are observed independently. The independence assumption is discussed in more detail and justified experimentally in chapter 11. Under this independence assumption, the probability that a world w exists is given by:

$$P(w) = \prod_{t \in I} (\prod_{x \in t} P(x \in t) \cdot \prod_{x \notin t} (1 - P(x \in t)))$$

For example, the probability of world 5 in figure 10.1(c) is $P(Game \in t_A) * (1 - P(Music \in t_A)) * P(Music \in t_B) * (1 - P(Video \in t_B)) = 1.0 * 0.8 * 0.7 * 0.6 = 0.336$.

In the general case, the occurrence of items may be dependent. For example, the

decision to purchase a new music video DVD may mean they are unlikely to purchase a music CD by the same artist. Alternatively, some items must be bought together. If these conditional probabilities are known, they can be used in the methods in this thesis. For example, the probability that both a video and music are purchased by customer B is $P(\{Video, Music\} \in t_B) = P(Video \in t_B) * P(Music \in t_B | Video \in t_B)$.

10.1.2 Problem Definition

An itemset is a *frequent itemset* if it occurs in at least *minSup* transactions, where *minSup* is a user specified parameter. In uncertain transaction databases however, the support of an itemset is uncertain; it is defined by a discrete probability distribution function (p.d.f). Therefore, each itemset has a *frequentness probability*[3] – the probability that it is frequent (defined formally in definition 10.10). This chapter focuses on the problem of efficiently calculating this p.d.f. (called the *support probability distribution function* and defined formally in definition 10.8) and extracting all *probabilistic frequent itemsets:*

Definition 10.4 (Probabilistic Frequent Itemset)**.** A *Probabilistic Frequent Itemset* (PFI) is an itemset with a *frequentness probability* of at least τ.

The parameter τ is the user specified minimum confidence in the frequentness of an itemset. If τ is set close to 1 then the user is interested only in itemsets that have a very high probability of being frequent, while a small value for τ (close to 0) would lead to results that also include itemsets which are frequent in very few possible worlds – that is, that have a very low probability of being frequent.

The problem may now be defined as follows:

Definition 10.5 (Probabilistic Frequent Itemset Mining)**.** Given an uncertain transaction database T, a minimum support scalar *minSup* and a frequentness probability threshold τ, *Probabilistic Frequent Itemset Mining (PFIM)* problem is to find all *probabilistic frequent itemsets.*

10.1.3 Contributions

This chapter makes the following contributions:

[3] Frequentness is the rarely used word describing the property of being frequent.

- It proposes a probabilistic framework for frequent itemset mining in uncertain transaction databases, based on the possible worlds model. Furthermore, it proposes the probabilistic frequent itemset mining (PFIM) problem.

- It presents a dynamic computation method for computing the probability that an itemset is frequent (the frequentness probability), as well as the entire probability distribution function of the support of an itemset, in $O(|T|)$ time[4]. Without this technique, it would run in exponential time in the number of transactions. Using this approach, the algorithm has the same time complexity as methods based on the expected support [25, 26, 58] but yields much better effectiveness.

- It proposes an algorithm – ProApriori – to mine all itemsets that are frequent with a probability of at least τ. This chapter also proposes an additional algorithm that incrementally outputs the probabilistic frequent itemsets in the order of their frequentness probability. This ensures that itemsets with the highest probability of being frequent are output first. This has two additional advantages; first, it makes the approach free of the parameter τ. Secondly, it solves the top k itemsets problem in uncertain databases.

10.1.4 Organisation

The remainder of this chapter is organised as follows: Section 10.2 surveys related work. Section 10.3 presents the probabilistic support framework. Section 10.4 shows how to compute the frequentness probability in $O(|T|)$ time. Section 10.5 presents ProApriori – a probabilistic frequent itemset mining algorithm. Section 10.6 presents the incremental algorithm. Experiments are presented in section 10.7 and this chapter concludes in section 10.8.

10.2 Related Work

There is a large body of research on Frequent Itemset Mining (FIM), a survey can be found in [43]. Recall also that section 4.3 provided an overview of FIM. However, very little work addresses FIM in uncertain databases [25, 26, 58]. Indeed, the problem is a recent one. The approach proposed by Chui et. al [26] computes the expected support of itemsets by summing all itemset probabilities in their U-Apriori algorithm. Later, in [25], they additionally proposed a probabilistic filter in order

[4] Assuming *minSup* is a constant.

to prune candidates early. In [58], the UF-growth algorithm is proposed. Like U-Apriori, UF-growth computes frequent itemsets by means of the expected support, but it uses the FP-tree [48, 47] approach in order to avoid expensive candidate generation. In contrast to the probabilistic approach in this chapter, itemsets are considered frequent if the expected support exceeds *minSup*. The main drawback of this estimator is that information about the uncertainty of the expected support is lost; [25, 26, 58] ignore the number of possible worlds in which an itemsets is frequent. [114] proposes exact and sampling-based algorithms to find likely frequent items in streaming probabilistic data. However, they do not consider itemsets with more than one item. Finally, except for [96], existing FIM algorithms assume binary valued items which precludes simple adaptation to uncertain databases. The approach in this thesis is the first that is able to find frequent itemsets in an uncertain transaction database in a probabilistic way.

Existing approaches in the field of uncertain data management and mining can be categorized into a number of research directions. Most related to the work in this chapter are the two categories "*probabilistic databases*" [17, 77, 79, 14] and "*probabilistic query processing*" [32, 54, 109, 83].

The uncertainty model used in this chapter is very close to the model used for probabilistic databases. A probabilistic database denotes a database composed of relations with uncertain tuples [32], where each tuple is associated with a probability denoting the likelihood that it exists in the relation. This model, called "*tuple uncertainty*", adopts the possible worlds semantics [14]. A probabilistic database represents a set of possible "certain" database instances (worlds), where a database instance corresponds to a subset of uncertain tuples. Each instance (world) is associated with the probability that the world is "true". The probabilities reflect the probability distribution of all possible database instances. In the general model description [79], the possible worlds are constrained by rules that are defined on the tuples in order to incorporate object (tuple) correlations. The ULDB model proposed in [17], which is used in *Trio*[9], supports uncertain tuples with alternative instances which are called x-tuples. Relations in ULDB are called x-relations containing a set of x-tuples. Each x-tuple corresponds to a set of tuple instances which are assumed to be mutually exclusive, i.e. no more than one instance of an x-tuple can appear in a possible world instance at the same time. Probabilistic top-k query approaches [83, 109, 77] are usually associated with uncertain databases using the tuple uncertainty model. The approach proposed in [109] was the first approach able to solve probabilistic queries efficiently under tuple independency by means of dynamic programming techniques. This chapter adopts the dynamic programming technique for the efficient computa-

tion of probabilistic frequent itemsets (PFIs).

Another uncertainty model also exists, called *attribute uncertainty* [24]. In this model, each tuple is assumed to be "certainly" existent, but their attributes are uncertain. Therefore, each attribute is instantiated by a range of values associated with a probability distribution. This model is often used in the context of probabilistic similarity queries over uncertain vector data [24, 54].

While managing uncertain data has been studied for a considerable time [115], recently there has been an increasing interest in algorithms and applications on uncertain data. [8, 115] provide surveys and categorise the three main research areas in this field: Modeling uncertain data, which considers the process of capturing the uncertainties in the data while keeping the data useful for database management applications; uncertain data management / analysing uncertain data, which considers the issue of incorporating uncertain data semantics into database management system and problems such as query processing, joins and indexing; and mining uncertain data, which develops data mining techniques that take into account the uncertainty of the data. A tutorial on mining uncertain and probabilistic data may be found in [75]. The work in this chapter falls primarily into the third category, since it proposes a new approach to frequent itemset mining that explicitly and effectively deals with a database's uncertainty. The solution to the top-k probabilistic frequent itemset query falls into the second category, while the probabilistic framework for itemset mining based on possible world semantics falls into the first.

10.3 Probabilistic Frequent Itemsets

Recall that previous work was based on the expected support [25, 26, 58].

Definition 10.6. Given an uncertain transaction database T, the *expected support* $E(X)$ of an itemset X is defined as $E(X) = \sum_{t \in T} P(X \subseteq t)$.

Considering an itemset frequent if its expected support is above *minSup* has a major drawback. Uncertain transaction databases involve uncertainty concerning the support of an itemset. It is important to consider this when evaluating whether an itemset is frequent or not. However, this information is forfeited when using the expected support approach. Returning to the example shown in figure 10.2, the expected support of the itemset $\{D\}$ is $E(\{D\}) = 3.0$. The fact that $\{D\}$ occurs for certain in one transaction, namely in t_2, and that there is at least one possible world

Notation	Description / Definition
W	Set of all possible worlds, $W = \{w_1, w_2, ...w_{\|W\|}\}$
w or w_i	Possible world instance $w \in W$
T	Uncertain transaction database (UTB) $T = \{t_1, t_2, ..., t_{\|T\|}\}$
t or t_i	Uncertain transaction $t \in T$
I	Set of all items
X	Itemset $X \subseteq I$
x	Item $x \in I$, $x \in X$
$S(X, w)$	Support of X in world w
$P(w)$	Probability that world w exists.
$P_i(X)$	Probability that the support of X is exactly i. The *support probability.*
$P_{\geq i}(X)$	Probability that the support of X is *at least* i. When $i = minSup$, this is the *frequentness probability*.
$P_{i,j}(X)$	Probability that i of the first j transactions contain X
$P_{\geq i,j}(X)$	Probability that *at least* i of the first j transactions contain X

Figure 10.3: Summary of notations.

where D occurs in five transactions are ignored when using the expected support in order to evaluate the frequency of an itemset. Indeed, suppose $minSup = 3$; do we call $\{D\}$ frequent? And if so, how certain can we even be that $\{D\}$ is frequent? By comparison, consider itemset $\{G\}$. This also has an expected support of 3, but its presence or absence in transactions is more certain. It turns out that the probability that $\{D\}$ is frequent is 0.7 and the probability that G is frequent is 0.91. While both have the same expected support, we can be quite confident that $\{G\}$ is frequent, in contrast to $\{D\}$. An expected support based technique does not differentiate between the two.

The confidence with which an itemset is frequent is very important for interpreting uncertain itemsets in a meaningful way. In order to address this problem, this section formally introduces the concept of probabilistic frequent itemsets (PFIs).

10.3.1 Probabilistic Support

In uncertain transaction databases, the support of an item or itemset cannot be represented by a unique value, but must be represented by a discrete probability distribution.

Definition 10.7. Given an uncertain transaction database T and the set W of

possible worlds (instantiations) of T, the *support probability* $P_i(X)$ of an itemset X is the probability that X has the support i. Formally,

$$P_i(X) = \sum_{w_j \in W, (S(X,w_j)=i)} P(w_j)$$

where $S(X, w_j)$ is the support of X in world w_j.

Intuitively, $P_i(X)$ denotes the probability that the support of X is exactly i . The support probabilities associated with an itemset X for different support values form the *support probability distribution* of the support of X.

Definition 10.8. The *probabilistic support* of an itemset X in an uncertain transaction database T is defined by the support probabilities of X ($P_i(X)$) for all possible support values $i \in \{0, ..., |T|\}$. This probability distribution is called *Support Probability Distribution Function* (SPDF) . The following statement holds: $\sum_{0 \leq i \leq |T|} P_i(X) = 1.0$.

Returning to the example of figure 10.2, figure 10.4(a) shows the support probability distribution of itemset $\{D\}$.

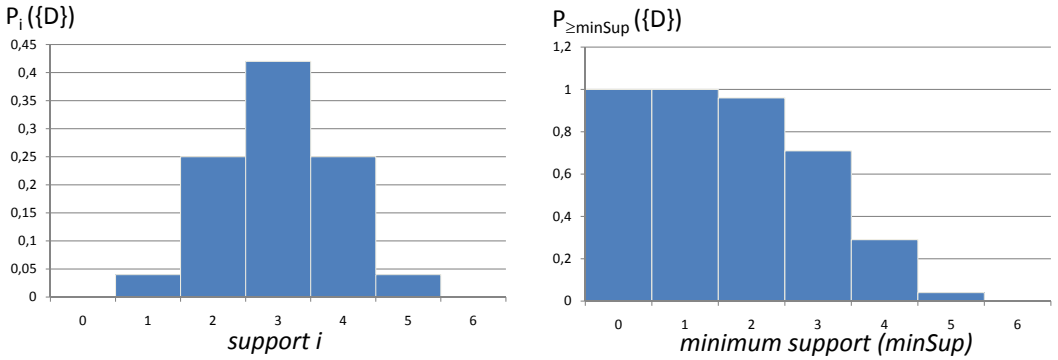
The number of possible worlds $|W|$ that need to be considered for the computation of $P_i(X)$ is extremely large. In fact, we have $O(2^{|T|\cdot|I|})$ possible worlds, where $|I|$ denotes the total number of items. In the following, this chapter shows how to compute $P_i(X)$ without materializing all possible worlds.

Lemma 10.9. For an uncertain transaction database T with mutually independent transactions and any $0 \leq i \leq |T|$, the support probability $P_i(X)$ can be computed as follows:

$$P_i(X) = \sum_{S \subseteq T, |S|=i} \left(\prod_{t \in S} P(X \subseteq t) \cdot \prod_{t \in T-S} (1 - P(X \subseteq t)) \right) \tag{10.1}$$

Note that the transaction subset $S \subseteq T$ contains exactly i transactions.

Proof. The transaction subset $S \subseteq T$ contains i transactions. The probability of a world w_j where all transactions in S contain X and the remaining $|T-S|$ transactions



(a) Support probability distribution of $\{D\}$ (b) Frequentness probabilities of $\{D\}$

Figure 10.4: Probabilistic support of itemset $X = \{D\}$ in the uncertain database of figure 10.2.

do not contain X is $P(w_j) = \prod_{t \in S} P(X \subseteq t) \cdot \prod_{t \in T-S}(1 - P(X \subseteq t))$. The sum of the probabilities according to all possible worlds fulfilling the above conditions corresponds to the equation given in definition 10.7. □

10.3.2 Frequentness Probability

Recall that the PFIM problem introduced in this chapter considers the *probability* that an itemset is frequent.

Definition 10.10. Let T be an uncertain transaction database and X be an itemset. $P_{\geq i}(X)$ denotes the probability that the support of X is *at least* i, i.e. $P_{\geq i}(X) = \sum_{k=i}^{|T|} P_k(X)$. For a given minimal support $minSup \in \{0, \ldots, |T|\}$, the probability $P_{\geq minSup}(X)$, called the *frequentness probability* of X, denotes the probability that the support of X is at least $minSup$.

Figure 10.4(b) shows the frequentness probabilities of $\{D\}$ for all possible $minSup$ values in the database of figure 10.2. For example, the probability that $\{D\}$ is frequent when $minSup = 3$ is approximately 0.7, while its frequentness probability when $minSup = 4$ is approximately 0.3.

The intuition behind $P_{\geq minSup}(X)$ is to show how confident one can be that an itemset is frequent. With this policy, the frequentness of an itemset becomes subjective and the decision about which candidates should be reported to the user depends on the application. Hence, this chapter uses the minimum frequentness probability τ as a user defined parameter. Some applications may need a low τ,

while in other applications only highly confident results should be reported (high τ).

In the possible worlds model, $P_{\geq i}(X) = \sum_{w_j \in W:(S(X,w_j)\geq i)} P(w_j)$. This can be computed according to Equation 10.1 by

$$P_{\geq i}(X) = \sum_{S \subseteq T, |S| \geq i} (\prod_{t \in S} P(X \subseteq t) \cdot \prod_{t \in T-S} (1 - P(X \subseteq t))). \tag{10.2}$$

Hence, the frequentness probability can be calculated by enumerating all possible worlds satisfying the *minSup* condition through the direct application of Equation 10.2. This naive approach is very inefficient however and can be sped up significantly. First, note that typically $minSup << |T|$ and the number of worlds with support i is at most $\binom{|T|}{i}$. Hence, enumeration of all worlds w in which the support of X is greater than *minSup* is much more expensive than enumerating those where the support is less than *minSup*. Using the following easily verified lemma, the frequentness probability can be computed exponentially in $minSup << |T|$.

Lemma 10.11. $P_{\geq i}(X) = 1 - \sum_{S \subseteq T:|S|<i} (\prod_{t \in S} P(X \subseteq t) \cdot \prod_{t \in T-S} (1 - P(X \subseteq t)))$.

Despite this improvement, the complexity of the above approach, called **Basic** in the experiments, is still exponential with respect to the number of transactions. Section 10.4 describes this can be reduced to linear time.

10.4 Efficient Computation of Probabilistic Frequent Itemsets

This section presents the dynamic programming approach, which avoids the enumeration of possible worlds in calculating the frequentness probability and the support distribution. It is based on the Poisson binomial recurrence. This section also presents probabilistic filter and pruning strategies which further improve the run time.

10.4.1 Efficient Computation of Probabilistic Support

The key to calculating the frequentness probability efficiently is to consider the problem in terms of sub-problems. First, appropriate definitions are required;

Definition 10.12. The probability that i of j transactions contain itemset X is

$$P_{i,j}(X) = \sum_{S \subseteq T_j : |S| = i} (\prod_{t \in S} P(X \subseteq t) \cdot \prod_{t \in T_j - S} (1 - P(X \subseteq t)))$$

where $T_j = \{t_1, ..., t_j\} \subseteq T$ is the set of the first j transactions. Similarly, the probability that *at least* i of j transactions contain itemset X is

$$P_{\geq i,j}(X) = \sum_{S \subseteq T_j : |S| \geq i} (\prod_{t \in S} P(X \subseteq t) \cdot \prod_{t \in T_j - S} (1 - P(X \subseteq t)))$$

Note that $P_{\geq i,|T|}(X) = P_{\geq i}(X)$, the probability that at least i transactions in the entire database contain X. The key idea is to split the problem of computing $P_{\geq i,|T|}(X)$ into smaller problems $P_{\geq i,j}(X)$, $j < |T|$. This can be achieved as follows. Given a set of j transactions $T_j = \{t_1, ..., t_j\} \subseteq T$, if we assume that transaction t_j contains itemset X, then $P_{\geq i,j}(X)$ is equal to the probability that at least $i - 1$ transactions of $T_j \backslash \{t_j\}$ contain X. Otherwise, $P_{\geq i,j}(X)$ is equal to the probability that at least i transactions of $T_j \backslash \{t_j\}$ contain X. By splitting the problem in this way, the recursion in lemma 10.13 can be used to compute $P_{\geq i,j}(X)$ by means of the paradigm of dynamic programming.

Lemma 10.13. $P_{\geq i,j}(X) =$

$$P_{\geq i-1,j-1}(X) \cdot P(X \subseteq t_j) + P_{\geq i,j-1}(X) \cdot (1 - P_j(X \subseteq t_j))$$

where

$$P_{\geq 0,j}(X) = 1 \ \forall . 0 \leq j \leq |T|, \ P_{\geq i,j} = 0 \ \forall . i > j$$

The above dynamic programming scheme is an adaption of a technique previously used in the context of probabilistic top-k queries by Kollios et. al [109].

Proof. $P_{\geq i,j}(X) = \sum_{k=i}^{j} P_{k,j}(X) \overset{[Kollios\ et\ al]}{=}$

$\sum_{k=i}^{j} P_{k-1,j-1}(X) \cdot P(X \subseteq t_j) + \sum_{k=i}^{j} P_{k,j-1}(X) \cdot (1 - P(X \subseteq t_j)) \overset{[P_{\geq i,j} = 0 \ \forall . i > j]}{=} P(X \subseteq t_j) \cdot \sum_{k=i}^{j-1} P_{k-1,j-1}(X) + \cdot (1 - P(X \subseteq t_j)) \cdot \sum_{k=i}^{j-1} P_{k,j-1}(X) = P(X \subseteq t_j) \cdot P_{\geq i-1,j-1}(X) + (1 - P(X \subseteq t_j)) \cdot P_{\geq i,j-1}(X)$. □

Using this result, it is possible to efficiently compute the frequentness probability of itemset X by calculating the cells shown in figure 10.5, where the entry in the

ith row and jth column is $P_{\geq i,j}(X)$. According to lemma 10.13, the probabilities $P_{\geq i-1,j-1}(X)$ and $P_{\geq i,j-1}(X)$ are required to compute $P_{\geq i,j}(X)$. That is, the entry to the left and the entry to the lower left of $P_{\geq i,j}(X)$. Since by definition $P_{\geq 0,j}(X) = 1 : 0 \leq j \leq |T|$ (it is certain that the support is at least 0) and $P_{\geq i,j}(X) = 0 : i > j$ (the support can not be greater than the number of transactions), the computation begins by computing entry $P_{\geq 1,1}(X)$. $P_{\geq 1,j}(X)$ can then be computed by using the previously computed $P_{\geq 1,j-1}(X)$. $P_{\geq 1,j}(X)$ can in turn be used to compute $P_{\geq 2,j}(X)$ and so on. Note that since the target value is $P_{\geq minSup,|T|}(X)$, in each row i of the matrix in figure 10.5, j only needs to vary from i to $|T| - minSup + i$. Larger values of j are not required for the computation of $P_{minSup,|T|}$, and smaller values are not required either. This approach continues as shown by the dotted lines in figure 10.5 until $i = minSup$ and $j = |T|$ and we obtain $P_{\geq minSup,|T|}(X)$; the frequentness probability (definition 10.10).

Lemma 10.14. *The computation of the frequentness probability $P_{\geq minSup}$ requires at most $O(|T| * \text{minSup}) = O(|T|)$ time and at most $O(|T|)$ space.*

Proof. Using the dynamic computation scheme as shown in figure 10.5, the number of computations is bounded by the size of the depicted matrix. The matrix contains $|T| * minSup$ cells. Each cell requires an execution of the equation in lemma 10.13, which is performed in $O(1)$ time. Note that a matrix is used here for illustration purpose only. The computation of each probability $P_{i,j}(X)$ only requires information stored in the current line and the previous line to access the probabilities $P_{i-1,j-1}(X)$ and $P_{i,j-i}(X)$. Therefore, only these two lines (of length $|T| - minSup + 1$) need to be preserved requiring $O(|T|)$ space (actually, a trick can be used so that only one line is required). Additionally, the probabilities $P(X \subseteq t_j)$ have to be stored, resulting in a total of $O(|T|)$ space. □

10.4.1.1 Certainty Optimisation or "0-1-Optimisation"

It is possible to save computation time whenever an itemset is certain in a transactions. If a transaction $t_j \in T$ contains itemset X with a probability of zero, i.e. $P(X \subseteq t_j) = 0$, transaction t_j can be ignored for the frequentness probability computation because $P_{\geq i,j}(X) = P_{\geq i,j-1}(X)$ holds (lemma 10.13). Ignoring these transactions can be thought of as using a subset $T' \subset T$ of the transactions. Further, note that if $|T'|$ is less than $minSup$, then X can be pruned immediately since, by definition, $P_{\geq minSup,T'} = 0$ if $minSup > |T'|$. That is, there are not enough transactions left in which X could appear for the support to reach $minSup$. The dynamic

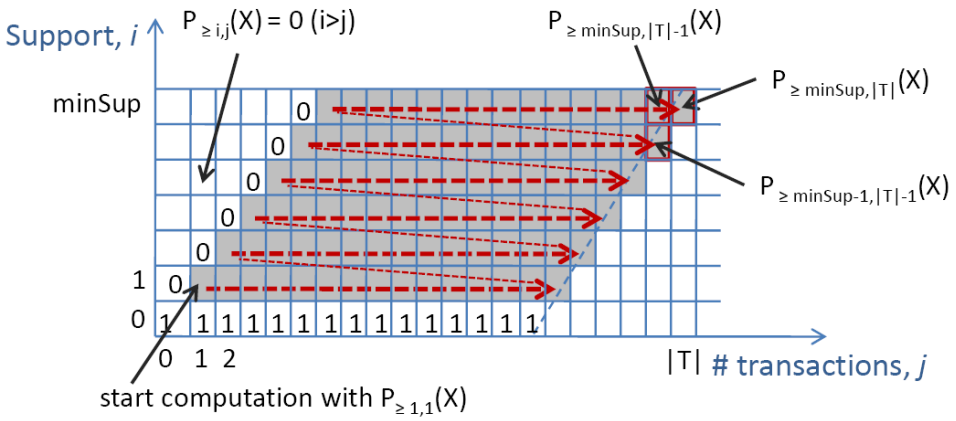


Figure 10.5: Dynamic computation scheme.

computation scheme can also omit transactions t_j where $P(X \subseteq t_j) = 1$ because then $P_{\geq i,j}(X) = P_{\geq i-1,j-1}(X)$. Therefore, if a transaction t_j contains X with a probability of 1, then the jth column can be omitted if *minSup* is reduced by one in order to compensate for this known-for-certain support.

As a consequence of these observations, the computation of the frequentness probability only has to consider uncertain entries in the database. This trick is called "certainty optimisation" or "0-1-optimization".

10.4.2 Probabilistic Filter Strategies

To further reduce the computational cost, probabilistic filter strategies are introduced which reduce the number of probability computations required. The probabilistic filter strategies exploit the following monotonicity criteria:

10.4.2.1 Monotonicity Criteria

If the minimum support required (i) is increased, then the frequentness probability of an itemset decreases.

Lemma 10.15. $P_{\geq i,j}(X) \geq P_{\geq i+1,j}(X)$.

Proof. $P_{\geq i+1,j}(X) = P_{\geq i,j}(X) - P_{i+1,j}(X) \leq P_{\geq i,j}(X)$ using definition 10.10. □

This result is intuitive since the predicate "the support is at least $i+1$" implies "the support is at least i" and hence the second event is at least as likely as the first.

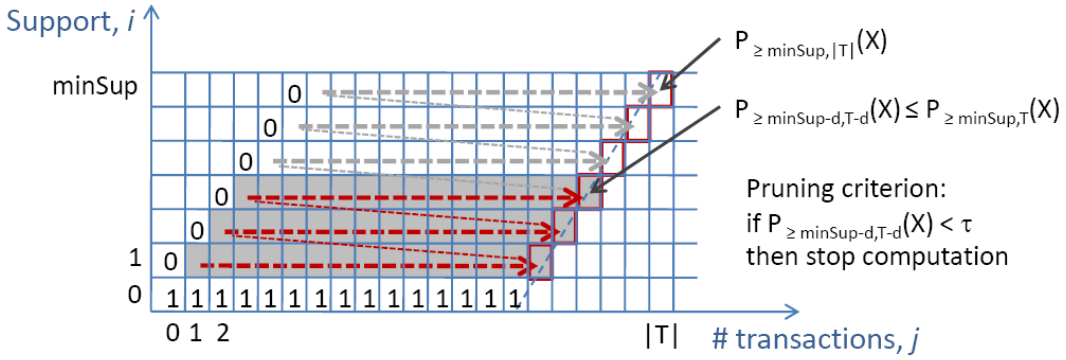


Figure 10.6: Visualisation of the pruning criterion. The computation can be pruned whenever a value $P_{\geq minSup-d,|T|-d}(X), 1 \leq d \leq minSup$ is less than τ.

The next criterion says that an extension of the uncertain transaction database leads to an increase of the frequentness probability of an itemset.

Lemma 10.16. $P_{\geq i,j}(X) \leq P_{\geq i,j+1}(X)$.

Proof. $P_{\geq i,j+1}(X) = P_{\geq i-1,j}(X) \cdot P(X \subseteq t_{j+1}) + P_{\geq i,j}(X) \cdot (1 - P(X \subseteq t_{j+1})) \overset{Lemma}{\geq} P_{\geq i,j}(X) \cdot P(X \subseteq t_{j+1}) + P_{\geq i,j}(X) \cdot (1 - P(X \subseteq t_{j+1})) = P_{\geq i,j}(X)$ using lemma 10.13 in the first $=$ and lemma 10.15 for the first $\geq$. □

The intuition behind this lemma is that one more transaction could increase the support of an itemset, since it could exist in that transaction. Putting these results together;

Lemma 10.17. $P_{\geq i,j}(X) \geq P_{\geq i+1,j+1}(X)$.

Proof. $P_{\geq i+1,j+1}(X) = P_{\geq i,j}(X) \cdot P(X \subseteq t_{j+1}) + P_{\geq i+1,j}(X)(1 - P(X \subseteq t_{j+1})) \leq P_{\geq i,j}(X) \cdot P(X \subseteq t_{j+1}) + P_{\geq i,j}(X)(1 - P(X \subseteq t_{j+1})) = P_{\geq i,j}$ using lemma 10.13 in the first $=$ and lemma 10.15 in the first $\leq$. □

The next section describes how these monotonicity criteria can be exploited to prune the frequentness probability computation.

10.4.2.2 Pruning Criterion

Lemma 10.17 can be used to quickly identify non-frequent itemsets. Figure 10.6 shows the dynamic programming scheme for an itemset X. Keep in mind that

the goal is to compute $P_{\geq minSup,|T|}(X)$. Lemma 10.17 states that the probabilities $P_{\geq minSup-d,|T|-d}(X), 1 \leq d \leq minSup$ (highlighted in figure 10.6), are conservative bounds of $P_{\geq minSup,|T|}(X)$. Thus, if any of the probabilities $P_{\geq minSup-d,|T|-d}(X)$, $1 \leq d \leq minSup$ is lower than the user specified parameter τ, then the computation can be immediately pruned since it is already clear that X cannot be a PFI.

10.5 Probabilistic Frequent Itemset Mining (PFIM)

The previous section section showed how to efficiently identify whether a given itemset X is a probabilistic frequent itemset (PFI). This section shows how to find all probabilistic frequent itemsets in an uncertain transaction database. Traditional frequent itemset mining is based on support pruning by exploiting the anti-monotonic property of support: $S(X) \leq S(Y)$ where $S(X)$ is the support of X and $Y \subseteq X$. In uncertain transaction databases however, support is defined by a probability distribution and itemsets are mined according to their frequentness probability. It turns out that the frequentness probability is anti-monotonic:

Lemma 10.18. $\forall Y \subseteq X : P_{\geq minSup}(X) \leq P_{\geq minSup}(Y)$. *In other words, all subsets of a probabilistic frequent itemset are also probabilistic frequent itemsets.*

Proof. $P_{\geq i}(X) = \frac{1}{|W|} \sum_{i=1}^{|W|} P(w_i) \cdot I_{S(X,w_i) \geq minSup}$, since the probability is defined over all possible worlds. Here, I_Z is an indicator variable that is 1 when $z = true$ and 0 otherwise. In other words, $P_{\geq i}(X)$ is the relative number of worlds in which $S(X) \geq minSup$ holds, where each occurrence is weighted by the probability of the world occurring. Since world w_i corresponds to a normal transaction database with no uncertainty, $S(X, w_i) \leq S(Y, w_i) \forall Y \subseteq X$ due to the anti-monotonicity of support. Therefore, $I_{S(X,w_i) \geq minSup} \leq I_{S(Y,W_i) \geq minSup} \forall i \in |W|, \forall Y \subseteq X$ and, thus, $P_{\geq i}(X) \leq P_{\geq i}(Y), \forall Y \subseteq X$. □

The contra-positive of lemma 10.18 can be used to prune the search space for PFIs. That is, if an itemset Y is not a PFI ($P_{\geq minSup}(Y) < \tau$), then all itemsets $X \supseteq Y$ cannot be probabilistic frequent itemsets either.

The first algorithm presented in this chapter is based on the combination of traditional frequent itemset mining methods and the PFI identification method described earlier. In particular, a probabilistic frequent itemset mining (PFIM) approach is proposed based on the Apriori algorithm ([11]). Like Apriori, the method iteratively generates the PFIs using a bottom-up strategy. Each iteration is performed in two

steps, a join step for generating new candidate PFIs and a pruning step for calculating the frequentness probabilities and identifying the PFIs from the set of candidates. In turn, these are used to generate candidates in the next iteration. Lemma 10.18 is exploited to prune the search space. The data set is stored in memory in a way that allows fast access to the $P(x_i \in t_j)$; in particular the vertical database layout [88] can be exploited effectively. This avoids the subset checking problem in the traditional Apriori algorithm. The algorithm is called ProApriori in this thesis.

10.6 Incremental Probabilistic Frequent Itemset Mining (I-PFIM)

Probabilistic frequent itemset mining (PFIM) allows the user to control the confidence of the results using τ. However, since the number of results also depends on τ, it may prove difficult for a user to correctly specify this parameter without additional domain knowledge. Furthermore, it can be expected that the user is interested in receiving the best results first. Therefore, this section shows how to efficiently solve the following problems, which do not require the specification of τ;

- *Top-k probabilistic frequent itemsets query:* return the k itemsets that have the highest frequentness probability, where k is specified by the user.
- *Incremental ranking queries:* successively return the itemsets with the highest frequentness probability, one at a time.

The problems are collectively called incremental PFIM (I-PFIM).

10.6.1 Incremental Probabilistic Frequent Itemset Mining Algorithm

The I-PFIM method computes the next most probable frequent itemset in each step, as shown in algorithm 10.1. The algorithm keeps an *Active Itemsets Queue (AIQ)* that is initialized with all one-item sets. The AIQ is sorted by frequentness probability in descending order. Without loss of generality, itemsets are represented in lexicographical order to avoid generating them more than once. In each iteration of the algorithm, i.e. each call of the *getNext()*-function, the first itemset X in the queue is removed. X is the next most probable frequent itemset because all other itemsets in the AIQ have a lower frequentness probability due to the order on the AIQ, and all of X's super-sets (which have not yet been generated) cannot have a

higher frequentness probability due to lemma 10.18. Before X is returned to the user, it is refined in a candidate generation step. In this step, super-sets of X are generated by adding single items x to the end of X. This is done in such a way that the lexicographical order of $X \cup x$ is maintained, thus avoiding duplicates. These are then added to the AIQ after their respective frequentness probabilities are computed (section 10.4). The user can continue calling the *getNext()*-function until he or she has all required results. Note that during each call of the *getNext()*-function, the size of the AIQ increases by at most $|I|$. The maximum size of the AIQ is $2^{|I|}$, which is no worse than the space required to sort the output of a non-incremental algorithm.

10.6.2 Top-k Probabilistic Frequent Itemsets Query

It is likely that relatively few top probabilistic frequent itemsets are required in practice. For instance, the store in Example 10.1 may want to know the top $k = 100$. Top-k most probable frequent itemsets queries can be efficiently computed by using algorithm 10.1 and constraining the length of the AIQ to $k - m$, where m is the number of highest frequentness probability items already returned. Not that this also provides a strict bound on the space required. Any itemsets that "fall off" the end of the AIQ can safely be ignored. The rational behind this approach is that for an itemset X at position p in the AIQ, $p - 1$ itemsets with a higher frequentness probability than X exist in the AIQ. Additionally, any of the m itemsets that have already been returned must have a higher frequentness probability. Consequently, the top-k algorithm constrains the size of the initial AIQ to k and reduces its size by one each time a result is reported. The algorithm terminates once the size of the AIQ reaches zero.

Algorithm 10.1 Incremental probabilistic frequent itemset mining algorithm.

```
//initialise
AIQ = new PriorityQueue
for each item x ∈ I
  AIQ.add([x, P≥minSup(x)]);
//return the next probabilistic frequent itemset
getNext() returns itemset X
  X =AIQ.removeFirst();
  for each x ∈ I \ X : x = lastInLexiographicalOrder(X ∪ x)
    AIQ.add([X ∪ x, P≥minSup(X ∪ x)]);
```

10.7 Experimental Evaluation

This section present efficiency and efficacy experiments. First, the algorithm and all optimisations and variations for computing the frequentness probability (sections 10.3 and 10.4) are evaluated and compared. Then, the performance and utility of the PFIM algorithm (ProApriori) and the incremental PFIM algorithm (sections 10.5 and 10.6) are evaluated.

Additional experiments can be found in chapter 13, where ProApriori is compared to algorithms developed in subsequent chapters on large, well known artificial and real databases.

10.7.1 Evaluation of the Frequentness Probability Calculations

The frequentness probability calculation methods were evaluated on several artificial data sets with varying database sizes $|T|$ (up to $10,000,000$) and densities. The *density* of an item denotes the expected number of transactions in which an item may be present (i.e. where its existence probability is in $(0, 1]$). The probabilities themselves were drawn from a uniform distribution. Note that the density is directly related to the degree of uncertainty. If not stated otherwise, a database consisting of $10,000$ uncertain transactions, 20 items, a density of 0.5 and frequentness probability threshold $\tau = 0.9$ were used.

The following notations are used for the frequentness probability calculation algorithms:

Basic: basic probability computation (section 10.3.2)

Dynamic: dynamic probability computation (section 10.4.1)

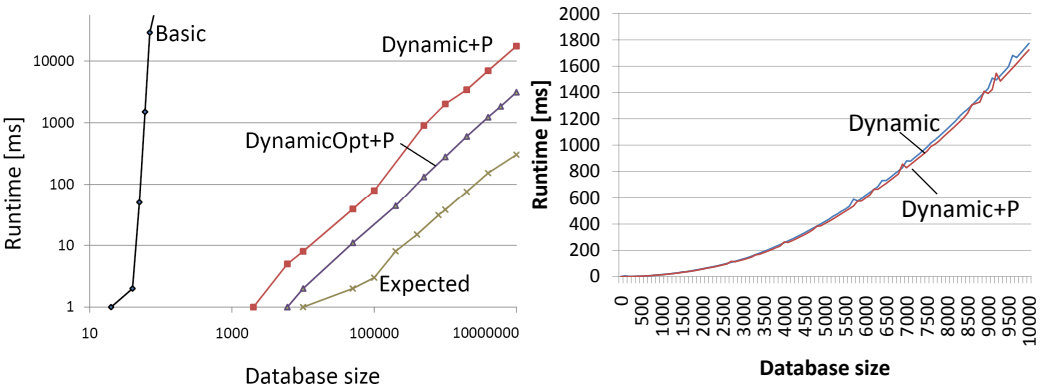
Dynamic+P: dynamic probability computation with pruning (section 10.4.2)

DynamicOpt: dynamic probability computation utilizing certainty optimisation; "0-1-optimization" (section 10.4.1) and

DynamicOpt+P: 0-1-optimized dynamic probability computation method with pruning.

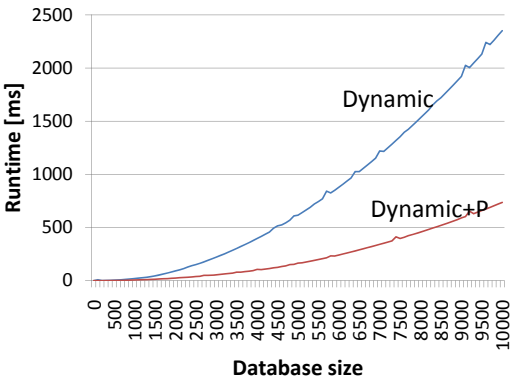
10.7.1.1 Scalability

Figure 10.7 shows the scalability of the frequentness probability calculation approaches when the number of transactions, $|T|$, are varied. The run time of the

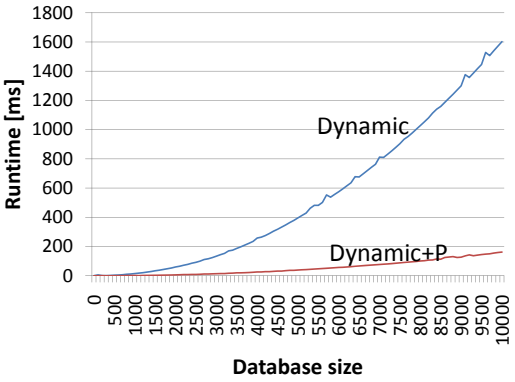


(a) $minSup = 10$

(b) $minSup = 25\%$



(c) $minSup = 50\%$



(d) $minSup = 75\%$

Figure 10.7: Run time evaluation of the frequentness probability computation algorithms with respect to the database size; $|T|$. Results shown for fixed $minSup = 10$ and for $minSup$ as percentage of $|T|$.

Basic approach increases exponentially in $minSup$ as explained in section 10.3.2, and is therefore not applicable for a $|T| > 50$ as can be seen in figure 10.7(a). The proposed approaches **Dynamic+P** and **DynamicOpt+P** scale linearly as expected when using a constant $minSup$ value (figure 10.7(a)). The 0-1-optimization has an impact on the run time whenever there is some certainty in the database. The performance gain of the pruning strategies depends on the $minSup$ value. In figures 10.7(b), 10.7(c) and 10.7(d) the scalability of **Dynamic** and **Dynamic+P** is shown for different $minSup$ values expressed as percentages of $|T|$. Note that the run time complexity of $O(|T| * minSup)$ becomes $O(|T|^2)$ if $minSup$ is chosen relative to the database size. Also, it can be observed that the higher the $minSup$, the higher the difference between **Dynamic** and **Dynamic+P**. This occurs since a higher $minSup$ causes the frequentness probability of itemsets to fall overall, thus allowing earlier pruning.

10.7.1.2 Effect of the Density

This section evaluates the effectiveness of the pruning strategy with respect to the density of the database. *minSup* is important here too, so results for different values are reported in figure 10.8. τ was 0.95 in these experiments. The pruning works well for data sets with low density and has no effect on the run time for higher densities. The reason is straightforward; the higher the density, the higher the probability that a given itemset is frequent and thus cannot be pruned. *minSup* also has an effect: a larger *minSup* decreases the probability that itemsets are frequent and therefore increases the number of computations that can be pruned. The break-even point between pruning and non-pruning in the experiments is when the density is approximately twice the *minSup* value, since, due to the method of creating the data sets, this corresponds to the expected support. At this value, all itemsets are expected to be frequent.

Overall, with reasonable parameter settings the pruning strategies achieve a significant speed-up for the identification of probabilistic frequent itemsets.

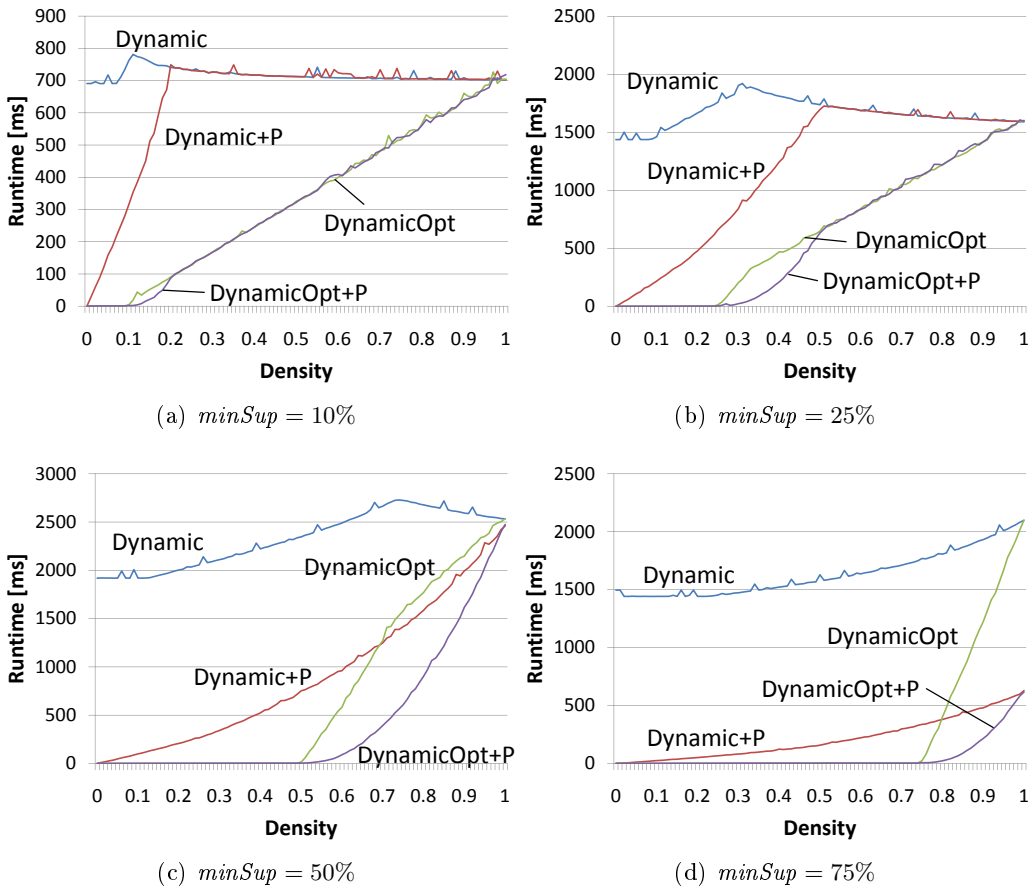
10.7.1.3 Effect of *minSup*

Figure 10.9 shows the influence of *minSup* on the run time when using different densities. The run time of **Dynamic** directly correlates with the size of the dynamic computation matrix (figure 10.5). A low *minSup* value leads to few matrix rows which need to be computed, while a high *minSup* value leads to a slim row width (see figure 10.5). The total number of matrix cells to be computed is the number of rows times their width; $minSup * (|T| - minSup + 1)$, which obtains it's maximum when $minSup = \frac{|T|+1}{2}$. As long as the *minSup* value is below the expected support value, the approach with pruning shows similar characteristics; in this case, almost all item(sets) are expected to be frequent. However, the speed-up due to the pruning rapidly increases for *minSup* above this break-even point.

10.7.2 Evaluation of the Probabilistic Frequent Itemset Mining Algorithms

This section evaluates ProApriori and the incremental PFM algorithm. Experiments were run on a subset of the real-world data set *accidents*[5], denoted by *ACC*. It consists of 340,184 transactions and 572 items whose occurrences in transactions

[5]The *accidents* data set [42] was derived from the Frequent Itemset Mining Data set Repository (http://fimi.cs.helsinki.fi/data/)



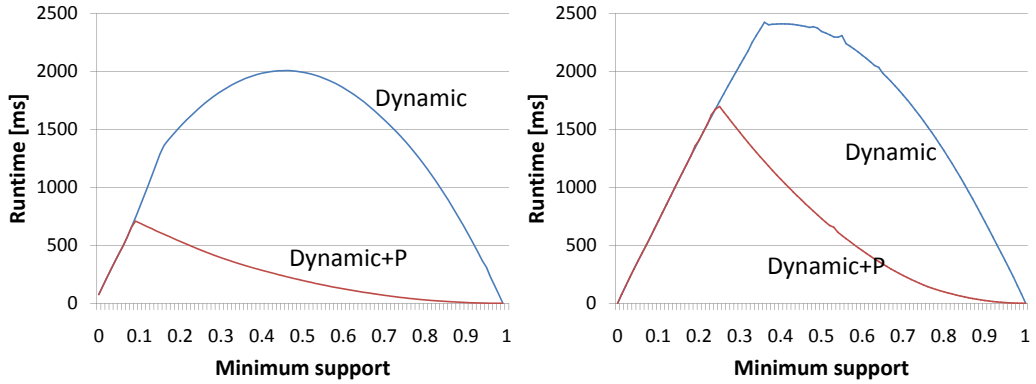
(a) $minSup = 10\%$ (b) $minSup = 25\%$

(c) $minSup = 50\%$ (d) $minSup = 75\%$

Figure 10.8: Run time evaluation of frequentness probability calculations with respect to the database's density.

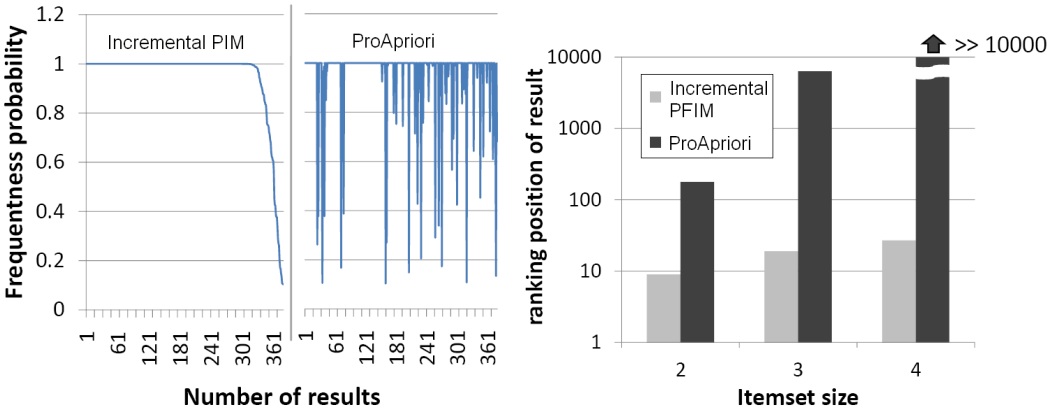
were randomized: With a probability of 0.5, each item appearing for certain in a transaction was assigned a value drawn from a uniform distribution in $(0, 1]$. In figure 10.10, **ProApriori** denotes the Apriori-based PFIM algorithm **Incremental PFIM** is the incremental probabilistic frequent itemset mining algorithm.

Top-k queries were performed on the first 10,000 transactions of ACC using $minSup = 500$ and $\tau = 0.1$ (specifying a τ is not necessary but if set, it can be used for pruning). Figure 10.10(a) shows the result of **Incremental PFIM**. Note that the frequentness probability of the resulting itemsets is monotonically decreasing. In contrast, **ProApriori** returns probabilistic frequent itemsets in the classic way; in descending order of their size, i.e. all itemsets of size one are returned first, etc. While both approaches return the same PFIs, **ProApriori** returns them in an arbitrary frequentness probability order, while **Incremental PFIM** returns the most relevant itemsets first.



(a) Density = 0.2 (b) Density = 0.5

Figure 10.9: Run time evaluation with respect to *minSup*.



(a) Output: AP vs. IP (b) Effectiveness of ranking queries

Figure 10.10: Effectiveness of the Incremental PFIM approach.

Next, ranking queries were performed on the first 100,000 itemsets (figure 10.10(b)). In this experiment, the aim was to find the m-itemset X with the highest frequency probability of all m-itemsets, where $m \in \{2, 3, 4\}$. The number of itemsets returned before the target X is returned was measured. It can be seen that the speed up factor for ranking (and thus top-k queries) is several orders of magnitude in comparison to a non-incremental approach, and increases exponentially in the length of requested itemset length. The reason is that a PFIM algorithm such as **ProApriori** must return all frequent itemsets of length $m-1$ before processing itemsets of length m, while **Incremental PFIM** is able to quickly rank itemsets in order of their frequentness probability, therefore leading to better quality results that are delivered to the user much earlier.

10.8 Conclusion

The Probabilistic Frequent Itemset Mining (PFIM) problem is to find itemsets in an uncertain transaction database that are (highly) likely to be frequent. The work in this chapter (and the paper it is based on, [18]) is the first to address this problem, and does so using a framework built on possible world semantics. This chapter theoretically and experimentally showed that the proposed dynamic computation technique is able to compute the exact support probability distribution and the frequentness probability of an itemset in linear time in the number of transactions. This is in comparison to the exponential run time of a non-dynamic approach. Furthermore, it was demonstrated that various probabilistic pruning strategies further improved the run time. In addition, a PFIM algorithm – ProApriori – was presented to mine all probabilistic frequent itemsets (PFIs). Finally, the incremental PFIM problem was introduced, where the most likely frequent itemsets are mined and reported incrementally. This was used to solve problems such as querying the top-k PFIs.

Chapter 11

Significant Frequent Itemset Mining

Frequent itemset mining in uncertain transaction databases (UTDBs) semantically and computationally differs from traditional techniques applied to standard "certain" databases since the support of an itemset is defined by a probability distribution rather than a single scalar.
This chapter introduces and solves the Significant Frequent Itemset Mining (SiFIM) problem for UTDBs. An itemset X is significantly frequent if, given a desired level of significance, we can reject the null hypothesis that its support is below *minSup*. This chapter formulates both a parametric and a non-parametric (exact) test to achieve this. The non-parametric approach is an adaptation of the PFIM method in chapter 10.
An incremental significant frequent itemset mining method is also proposed, which may help reduce the effects of the multiple tests problem. An extensive experimental analysis evaluates all methods. Furthermore, the independence assumption used in PFIM and SiFIM is validated and a demonstration of the the downsides of the Expected Frequent Itemset Mining (EFIM) method is provided.

11.1 Introduction

It is usually assumed that the items in a transaction are "certain", that is; an item is either present or absent. In practice this is not always the case – the presence of an item may be uncertain. Recall from section 10.1 that such situations may occur due to inherently noisy data, the addition of noise for privacy protection purposes [107] or through aggregation of records in order to produce purchase probabilities. Furthermore, data sets are generated from observations of a process and, even when the results of those observations are known for certain, they implicitly contain noise when the underlying process is noisy.

Dealing with uncertain databases is a difficult but interesting problem. Prior to the work in chapter 10 ([18]), existing approaches in the literature were based on the expected support, first introduced in [26]. Recall that in this method, itemsets are considered frequent if the expected support exceeds *minSup* [25, 26]. Also recall that this approach effectively returns an estimate of whether an object is frequent or not with no indication of how good this estimate is – in fact, an expected frequent itemset can be infrequent with high probability.

This chapter builds on chapter 10 and introduces the concept of *significant frequent itemsets*. A significant frequent itemset is an itemset where, given a desired level of significance, we can reject the null hypothesis that its support is below *minSup*. This chapter develops the theory and method for both a parametric and a non-parametric test for determining whether an arbitrary itemset is significantly frequent. By building on this, it introduces the first significant frequent itemset mining (SiFIM) method that can be used for uncertain, probabilistic or noisy data. The advantage of this approach is that the user can be confident that the reported itemsets are indeed frequent, thus greatly reducing the risk that frequent itemsets are reported in error. This can be achieved without much computation overhead in comparison to the expectation approach. The approach is also used to demonstrate the downsides of the expected frequent itemset approach; in particular, most expected frequent itemsets are insignificant and can occur by chance alone.

11.1.1 Problem Definition

An itemset is a *frequent itemset* if it occurs in at least *minSup* transactions, where *minSup* is a user specified parameter. In uncertain or noisy transaction databases however, an itemset's support is a probability distribution and in general, one cannot be sure whether an itemset is frequent or whether it just appears to be frequent by chance, due to the noise or uncertainty in the database.

Definition 11.1. A *Significant Frequent Itemset* (SFI) is an itemset where we can reject, at a desired significance level α, the null hypothesis that the support is less than *minSup*.

The significance level α is typically 0.05 or 0.01. Intuitively, a significant frequent itemset has a very high (statistically significant) probability of being frequent (*frequentness probability*). The problem definition is as follows:

Definition 11.2. Given an uncertain transaction database T, a minimum support scalar *minSup* and a significance level α, the *Significant Frequent Itemset Mining Problem* (SiFIM) is to find all *SFIs*.

The development of significance tests requires an appropriate probability model to derive the required approximate and exact distributions. The possible worlds model introduced in chapter 10 is used for this purpose. The reader may like to refer back to section 10.1.1 for an explanation and the definitions applying to this model, and figure 10.3 for a summary of the notation.

11.1.2 Contributions

This chapter makes the following contributions**:**

- It formally introduces and efficiently solves the Significant Frequent Itemset Mining (SiFIM) problem.
- A parametric significance test for finding significant frequent itemsets is developed, and its advantages and limitations are investigated. As a side effect, this approach can be adapted to approximately solve the probabilistic frequent itemset mining problem of chapter 10 in $O(|T|)$ time.
- An efficient non-parametric significance test is developed. No assumptions about the distribution of item and itemsets are made, leading to exact *p-value*s. Exact tests are usually much slower than their parametric counterparts. Indeed, a straightforward implementation would run in exponential time in the number of transactions $|T|$. However, based on the work in chapter 10, a method is developed that runs in $O(|T| \cdot minSup)$ time.
- All methods are evaluated experimentally. Furthermore, it is shown that despite the independence assumption made in this and previous work, dependent

itemsets can still be mined. The shortcomings of the expected support method is also demonstrated experimentally.

11.1.3 Organisation

The remainder of this chapter is organised as follows: Section 11.2 briefly surveys related work and puts the contributions in context. Section 11.3 introduces the model and significance tests. Section 11.3.1 discusses the independence assumption. Section 11.3.2 presents the parametric significance test, while section 11.3.3 presents the non parametric (exact) test. An incremental mining method, useful in overcoming the multiple tests problem, is discussed in section 11.4. Experiments are presented in section 11.5 and this chapter concludes in section 11.6.

11.2 Related Work

Recall that section 10.2 provided a discussion of work related to frequent itemset mining in uncertain and probabilistic databases. This section briefly covers work specific to significant itemset mining, of which there seems to be little.

[114] proposes exact and sampling-based algorithms to find likely frequent items in streaming probabilistic data. In [114], an efficient approach is presented to find significant frequent items (that is, itemsets of size one) in uncertain databases and is based on the possible worlds semantics and the *X-Relation* model. [114] also proposes sampling-based algorithms to find significantly frequent items in streaming data. The main restriction of [114] is that it is only applicable for itemsets of size one.

While it is a separate research problem and does not consider uncertain or probabilistic databases, several approaches have been proposed to define and measure the significance of association rules. For example, [98, 103] find significant association and classification rules based on Fisher's exact test. The approach proposed in [82] measures the significance of association rules via the chi-squared test of independence to evaluate correlations among items. Itemsets can be called significant if both the minimum support and minimum correlation criteria are met. Testing for significant correlations is a well-known statistical problem, and the reader is referred to to [55] which gives a closer insight into the theory. In [61] the chi-squared tests are used for pruning and summarizing association rules. In order to effectively prune and extract meaningful association rules, [87] presents three adaptive Apriori association rule mining methods. These methods are able to discover itemsets with low and

Notation	Description /
$p\text{-}value(X)$	The *p-value* of a significance test on whether X is frequent. $p\text{-}value(X) = 1 - P_{\geq minSup}(X)$.
$\hat{P}_i(X)$	The parametric approximation to the probability that the support of X is i
$\hat{P_{\geq i}}(X)$	The parametric approximation to the probability that the support of X is *at least* i
$\hat{P_{i,j}}(X)$	The parametric approximation to the probability that i of the first j transactions contain X
$\hat{P_{\geq i,j}}(X)$	The parametric approximation to the probability that *at least* i of the first j transactions contain X

Figure 11.1: Additional notation introduced in this chapter. Recall that figure 10.3 contains the basic notations required for itemset mining in probabilistic databases. The probabilities listed there are the exact probabilities.

high frequency. There are several further approaches to assessing the significance of itemsets, including methods using re-sampling-based permutation tests [68], methods using union-type bounds to estimate probability of an itemset under a random (Bernoulli) model [106] and methods based on generative models for transactions in the form of Itemset Generating Models (IGMs). These can be used to formally connect the process of frequent itemsets discovery with the learning of generative models [56]. In [33], the "significance" is measured by means of the ratio of actual-to-baseline frequencies based on a baseline frequency for each itemset. None of the above work is based on uncertain or probabilistic databases.

11.3 Significant Frequent Itemsets

Recall from section 10.3.1 that, given an uncertain transaction database T and the set W of possible worlds (instantiations) of T, the *support probability* $P_i(X)$ of an itemset X is the probability that X has the support i (definition 10.7). Formally,

$$P_i(X) = \sum_{w_j \in W, (S(X,w_j)=i)} P(w_j)$$

where $S(X, w_j)$ is the support of X in world w_j and $P(w_j)$ is the probability that world w_j exists. Recall that the notations are summarised in figure 10.3. Figure 11.1 summarises additional notation used in this chapter. The support probabilities associated with an itemset X for different support values form the *support probability distribution* of X (definition 10.8).

In order to test whether an itemset is significantly frequent, the following methodology is used. The *Null Hypothesis* states that an itemset X is not frequent under the assumption that the items of X are mutually independent. The probability that the null hypothesis holds is then calculated – $p\text{-}value(X)$. The null hypothesis can be rejected if $p\text{-}value(X)$ is low enough. More formally, we have the following two hypotheses:

- **Null hypothesis** H_0: the support of itemset X is less than $minSup$.
- **Alternative hypothesis** H_1: the support of itemset X is at least $minSup$.

The null hypothesis is rejected if the probability is at most α that the itemset X has a support value at most $minSup - 1$. Therefore;

Definition 11.3. The $p\text{-}value$ for the significance test on an itemset X under H_0 is $p\text{-}value(X) = P_{<minSup}(X) := \sum_{k=0}^{minSup-1} P_k(X)$.

H_0 is rejected for itemset X in favour of H_1 if $p\text{-}value(X) < \alpha$. If H_0 is rejected, X is called a *Significant Frequent Itemset* (definition 11.1).

11.3.1 Discussion of the Independence Assumption

In previous literature, independence between items is assumed [25, 26] and is justified by the assumption that the items are observed independently. This chapter considers this issue more thoroughly.

Under the independence assumption, the probability that an itemset X is contained in a transaction $t \in T$ is

$$P(X \subseteq t) = \Pi_{x \in X} P(x \in t).$$

If dependency information among items is supplied, then the corresponding conditional probabilities can be used in the method considered in this chapter[1]. However,

[1] For example, assume that two items x and y are mutually dependent and this dependency is known in advance. Then the probability that the itemset $X = \{x, y\}$ is contained in a transaction $t \in T$ is

$$P(X \subseteq t) = P(y \in t | x \in t) \cdot P(x \in t),$$

where $P(y \in t | x \in t)$ is the conditional probability that item y is in transaction t under the assumption that item x is in t.

it is not practical or necessary. By definition, an uncertain transaction databases lacks the ability to represent dependency information since it records the existence probability per item per transaction (see definitions 10.2 and 10.3). Even if the definition were extended, two problems arise: First, dependency information is difficult to collect. Secondly, capturing it would require exponential space, since there are an exponential number of conditional probabilities amongst a set of items. Hence, in practice, we have little choice but to assume independence.

The significance test based on the independence assumption helps identify dependencies between items that are inherent in the data. For example, if customers typically buy a set of products together and do so frequently, then one might expect a dependency between those products for that customer. It actually makes sense that under the null hypothesis, the occurrence of items in transactions are assumed to be independent for the purpose of calculating the *p-value*, since the significance test methodology involves assuming no relationship between items, but proving otherwise.

Finally, and perhaps most importantly, the experimental evaluation in section 11.5.3 shows that the dependencies between items are found accurately, despite the use of the independence assumption. This validates the assumption in practice.

In addition to the assumption that uncertain items in a transaction are mutually independent, it is also assumed that uncertain transactions are mutually independent. This is valid in practice. For instance, in a UTDB containing aggregated customer data, this means that a decision by one customer has no influence on another customers decisions. In transaction databases without such aggregation, it simply means the transactions are independent.

11.3.2 Parametric Computation of the p-value

In the possible world model, the occurrence of itemsets are implicitly modeled as Bernoulli random variables, with the existence probability as the mean of these. That is, the existence probability "generates" the possible worlds according to the Bernoulli distribution. Conversely, for the parametric computation the existence probability is treated as the expected number of worlds in which the itemset is present.

Therefore, in the model for the parametric test, the occurrence of an itemset X in transaction t is a Bernoulli random variable with an expected value of $P(X \subseteq t)$

and variance $P(X \subseteq t) \cdot (1 - P(X \subseteq t))$. Note that while these random variables are independent due to the independence of uncertain transactions, they are not identically distributed.

The support of an itemset X is simply the sum of these $|T|$ independent (but *not* identically distributed) Bernoulli random variables. Call this sum $S_{|T|}(X)$. Since the expectation of a sum is the sum of the expectations, and the variance of the sum of uncorrelated variables is the sum of the variances, the following holds:

$$\mu_X = E(S_{|T|}(X)) = \sum_{t \in T} P(X \subseteq t)$$

$$\sigma_X^2 = Var(S_{|T|}(X)) = \sum_{t \in T} P(X \subseteq t) \cdot (1 - P(X \subseteq t))$$

Under the Central Limit Theorem, provided $|T|$ is large enough, $S_{|T|}(X)$ converges to the Normal distribution. With a continuity correction, this provides a good approximation. Note that the number of transactions $|T|$ is very large in transaction databases. In summary:

Lemma 11.4. *The support probability distribution of an itemset X is approximated by the Normal distribution with mean μ_X and variance σ_X^2 as defined above. Therefore,*

$$\hat{P}_{\leq i}(X) = \frac{1}{\sigma_X \sqrt{2\pi}} \int_{-\infty}^{i+0.5} e^{-\frac{(x-\mu_X)^2}{2\sigma_X^2}}$$

where the $i + 0.5$ is the continuity correction to compensate for the fact that $S_{|T|}(X)$ is discrete.

The *p-value* is therefore $p\text{-}value(X) = \hat{P}_{<minSup}(X)$.

Since the cumulative Normal has no closed form solution, this work uses the Abromowitz and Stegun approximation [4] to evaluate it quickly. The result is a fast parametric significance test for determining whether an itemset is a significant frequent itemset.

Lemma 11.5. *The run time of the parametric test is $O(|T|)$*

Proof. The method requires only the computation of the mean, variance and then the Abromowitz and Stegun approximation to the cumulative normal distribution. □

While this parametric test works on average and converges as expected, its drawback is that it can lead to errors in comparison to the exact method for individual itemsets. These errors can be larger than α, which is problematic. Furthermore, it may not be strictly anti-monotonic when applied to itemset mining. In the next section, the non-parametric (exact) method is presented. The advantages of this are that there is no need to make any assumptions or arguments based on limiting distributions. The downside is that it takes longer to compute. By adapting the method in chapter 10 however, this chapter shows how to achieve it in $O(|T| \cdot minSup)$ time.

11.3.3 Non-Parametric Calculation of the (Exact) p-value

In order to calculate the exact (non-parametric) *p-value*, the possible worlds model is used. There are no additional assumptions to those in section 11.3.

Recall from section 11.3 that the support probability distribution was defined by the probabilities $P_i(X)$. From definition 10.7 we know that these can be calculated by enumerating the possible worlds $P(w)$. Recall that under the independence assumption, the probability that a w exists is given by:

$$P(w) = \prod_{t \in I} (\prod_{x \in t} P(x \in t) * \prod_{x \notin t} (1 - P(x \in t)))$$

To compute $p\text{-}value(X)$, it is possible to simply sum the probabilities of all the worlds where support of itemset X is at most i:

$$p\text{-}value(X) = P_{<minSup}(X) = \sum_{w \in W : (S(X,w) < i)} P(w)$$

Unfortunately, the number of possible worlds $|W|$ that need to be considered using this enumeration approach is large since there are $O(2^{|T| \cdot |I|})$ possible worlds, where I is the set of items.

Note that computing the *p-value* is equivalent to computing $P_{\geq minSup}(X)$ since $p\text{-}value(X) = P_{<minSup}(X) = 1 - P_{\geq minSup}(X)$. It is therefore possible to apply the results of chapter 10: $P_{\geq i}(X)$ can be computed very efficiently in $O(|T|)$ using an adaption of the Poisson Binomial Recurrence.

$$P_{\geq i}(X) = P_{\geq i,T}(X) = P_{\geq i-1,T \setminus t}(X) \cdot P(X \subseteq t) + P_{\geq i,T \setminus t}(X) \cdot (1 - P(X \subseteq t))$$

$$P_{\geq 0,T'}(X) = 1,\ P_{\geq i,T'}(X) = 0\ \forall .i > |T'| \forall .T' \subseteq T$$

where $P_{\geq i,T'}(X)$ denotes the probability that the support of itemset X is at least i in the set of transactions $T' \subseteq T$.

As a consequence of this adaptation of PFIM, it should also be clear that the SiFIM problem is anti-monotonic.

11.4 Incremental Significant Frequent Itemset Mining

The SiFIM approach allows the user to control the level of significance required by using the parameter α. However, since the number of results also depends on α, it may prove difficult for a user to correctly specify this parameter; depending on *minSup*, even a reasonable $\alpha = 0.01$ may yield too many results.

More importantly, if the user wishes to take the multiple tests problem into account to keep the false positive rate constant (according to their experimental conditions), for instance by adjusting α using the Bonferroni adjustment [3], then the number of itemsets *tested* is critical. When one performs more than a single hypothesis test, α can no longer be interpreted as the probability that the test reports a significant result by chance. The more tests one performs, the higher the likelihood that one of those tests will report a significant result by chance and therefore the lower the significance of the hypothesis that was labeled significant.

Solving the following problems do not require the specification of α and limit the effect of the multiple tests problem by allowing the user complete control over the number of significant itemsets mined. The number of itemsets tested (which enables adjustment for the multiple tests problem) can also be output.

- *Top-k significant frequent itemsets query:* return the k itemsets that are frequent at the highest level of significance, where k is specified by the user.
- *Incremental ranking queries:* successively return the itemsets in increasing order of their *p-value*. That is, return the most significant frequent itemsets one at a time.

Both these problems can be solved by adapting the methods in section 10.6. In particular, the *AIQ* is now sorted by the *p-value* of the corresponding SiFIMs in increasing order.

Please note that a complete treatment of the multiple tests problem and how to overcome it is beyond the scope of this chapter and depends on the users needs

and experimental setup. However, the Bonferroni adjustment is a commonly used method that is applicable to the current problem.

11.5 Experimental Evaluation

The evaluation begins by demonstrating the problems with using expected frequent itemsets in UTDBs, which contributes to the motivation for this chapter and indeed all the chapters in part IV of this thesis. Then, the efficacy of the parametric method is evaluated by comparing its calculated *p-values* to those of the exact method. While the parametric method is effective on average and converges, the convergence can sometimes be slow and errors larger than $\alpha = 0.05$ can occur. This motivates the exact method, which is a little slower. Subsequently, all methods are evaluated in terms of database properties and sensitivity to parameter settings. Then, the usefulness of the incremental significant frequent itemset mining algorithm is demonstrated using the exact method. Finally, it is demonstrated that the independence assumption does not prevent the method from finding dependent itemsets. This experiment therefore validates the independence assumption in part IV of this thesis.

The underlying itemset mining algorithm used is based on Apriori, as was the case in chapter 10. A number of experiments were performed on artificial data sets with varying database sizes and levels of uncertainty. The degree of uncertainty in is expressed by the "density" of uncertain items. The density denotes the relative number of transactions in which the items are uncertain, i.e. have a probability between zero and one. Unless otherwise stated, these probabilities were drawn from a uniform distribution. The real data sets is introduced when needed.

11.5.1 Expected vs. Significant Frequent Itemsets

Recall that prior to the work in this thesis, existing approaches dealing with itemset mining in UTDBs were based on expected support. This section demonstrates that mining expected frequent itemsets (EFI) returns many insignificant itemsets: While the itemsets have expected support above *minSup*, the probability that this is the case can often be so low that it can easily have occurred by chance alone. Indeed, it is even possible that an itemset with expected support above *minSup* has a greater probability of having support below *minSup* than above it! This can occur when the support probability distribution is skewed. Usually, with typical values for α, a

p-value	Expected Frequent Itemsets
Itemsets	253
Run time (ms)	6569

(a) Expected frequent itemsets.

	Significant Frequent Itemsets (Exact)		
p-value	0.05	0.01	0.001
Itemsets	56	17	1
Run time (ms)	48458	15084	11870

(b) Significant frequent itemsets using the exact method.

	Significant Frequent Itemsets (Parametric)		
p-value	0.05	0.01	0.001
Itemsets	51	14	1
Run time (ms)	710	119	82

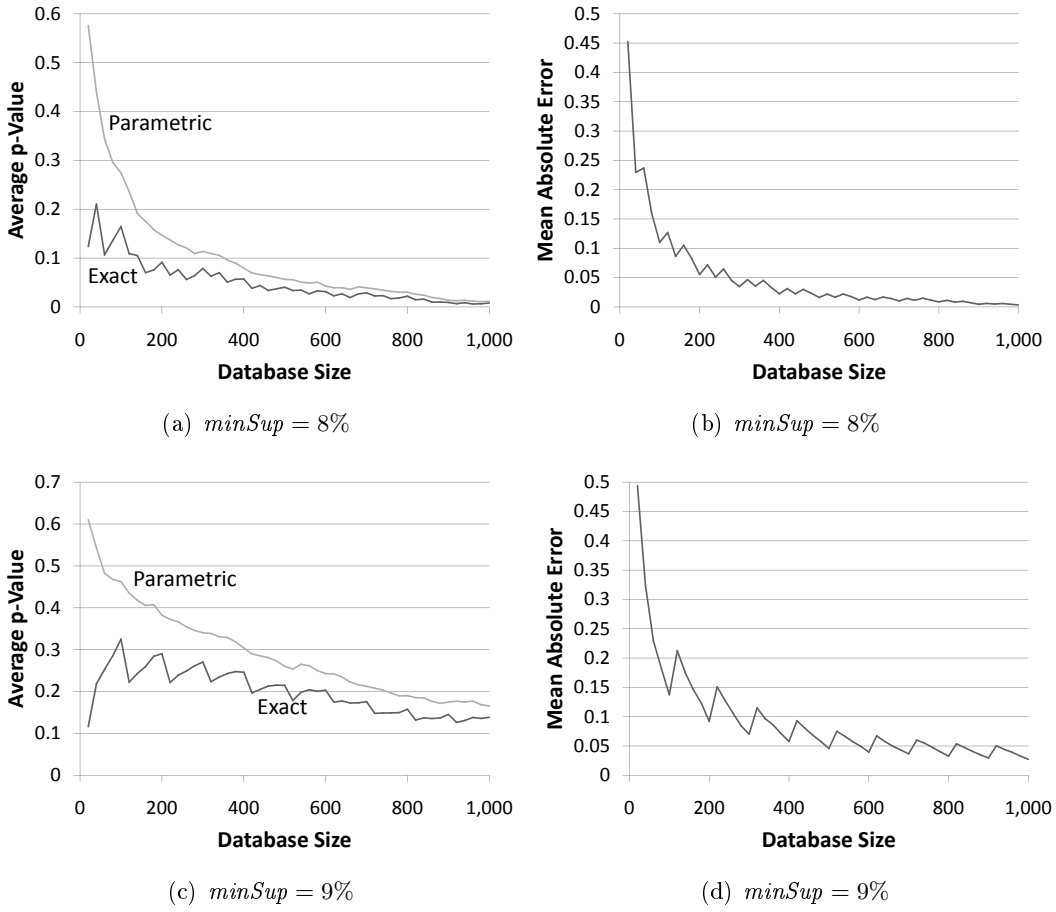
(c) Significant frequent itemsets using the parametric method.

Figure 11.2: Number of itemsets mined and run time of the expected frequent itemsets and significant frequent itemsets methods.

significant frequent itemset is also an expected frequent itemset, though the reverse does not hold.

A synthetic data set was used, consisting of $10,000$ transactions, 500 items, a density of 0.1 and $minSup = 500$. All expected and significant frequent itemsets were mined. As can be seen from figure 11.2, there were 253 expected frequent itemsets, but only 56 (22.1%) of these were significant frequent itemsets at the 0.05 level. At the 0.01 and 0.001 levels, only 17 (6.7%) and 1 (0.4%) were significant, respectively. Examining the results in more detail, it was found that among the expected frequent itemsets, some had *p-value*s of 0.48. That is, itemsets that, while reported to be frequent using EFI, are likely frequent only by chance. Furthermore, there were also itemsets with exactly the same expected support as these false positives but with a very low *p-value*.

Not only does the expected frequent itemset approach yield many false positives, these false positives also require it to examine more of the search space. For example, even though the parametric method takes longer per itemset (run time experiments are given below) than the expected support approach, overall it is faster since it finds only the high quality solutions.



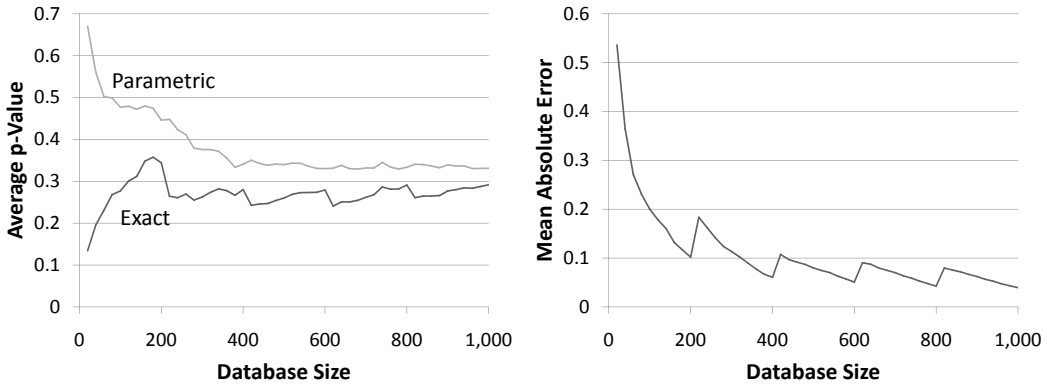
(a) $minSup = 8\%$ (b) $minSup = 8\%$

(c) $minSup = 9\%$ (d) $minSup = 9\%$

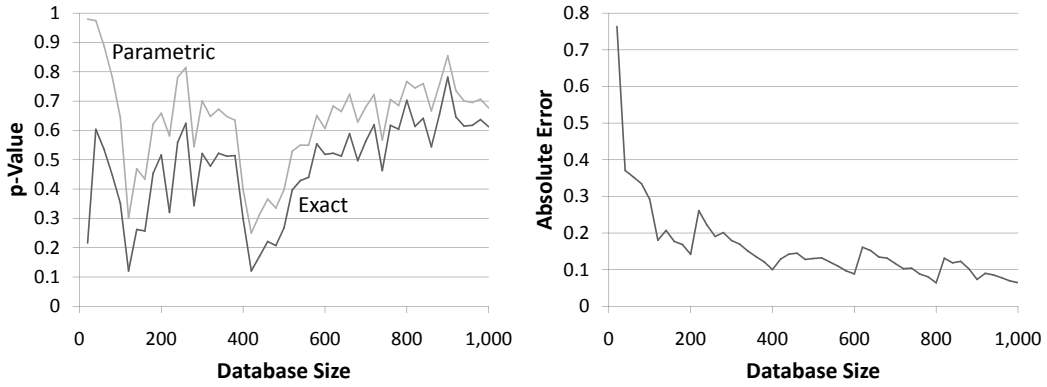
Figure 11.3: Convergence of the *p-value* on synthetic data sets (part 1). Continued in figure 11.4.

11.5.2 Evaluation of the Parametric Test

In these experiments, the *p-value* is calculated using the parametric and non-parametric methods. Experiments were performed on a synthetic and a real data set, as can be seen in figure 11.3. The synthetic data set consists of 1,000 transactions and 100 items, and was created with a density of 0.2. Figures 11.3(a) to 11.4(d) show results on the synthetic data set. The averages in Figures 11.3(a) to 11.4(b) are calculated over 100 randomisations of the data set. These figures show that the parametric approach converges, but it can take some time for this to happen and the errors can remain large – i.e. larger than typical significance levels. On average the *p-value* returned by the parametric method is higher than the exact value (this is not always the case for particular itemsets or databases) which results in false negatives rather than false positives. The effect of these differences on the overall itemset mining algorithm can be seen in figure 11.2, where the parametric method always returns



(a) $minSup = 9.5\%$ (b) $minSup = 9.5\%$

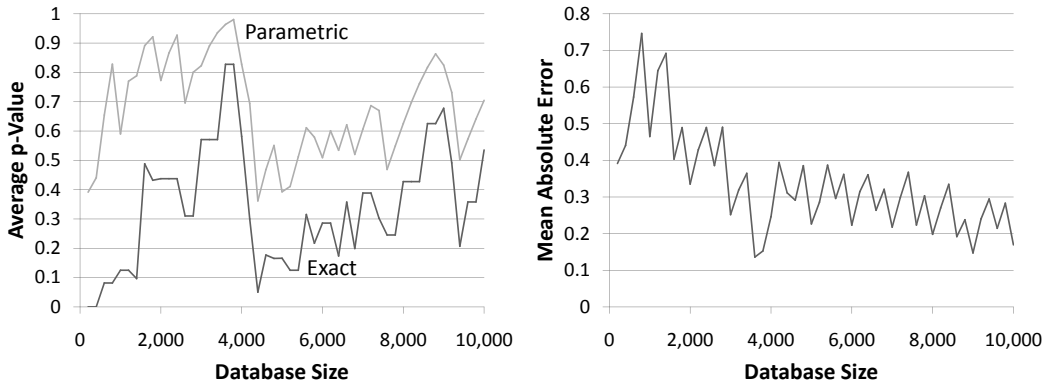


(c) Single item, $minSup = 9.5\%$ (d) Single item, $minSup = 9.5\%$

Figure 11.4: Convergence of the *p-value*on synthetic data sets (part 2).

fewer significant itemsets than the exact method. Figures 11.4(c) and 11.4(d) show one particular result (i.e. no averaging). As is to be expected, the error is greater when the convergence for specific itemsets is considered, compared to the average case.

Figures 11.5(a) and 11.5(b) show the average *p-value* and mean absolute error computed for a chosen item and averaged over 100 randomisations of the real data set. Here, the retail data set [21] was used. The first $10,000$ transactions were taken and randomised by converting the probabilities of half the (certain) items to a probability uniformly distributed in $[0, 1)$. The parametric method does not perform well on real data sets. This example was particularly bad. Overall, the parametric method converges and usually generates reasonable results (on average) once there are many transactions. Its drawbacks motivate the exact method.



(a) (b)

Figure 11.5: Real (retail) database, $minSup = 2$

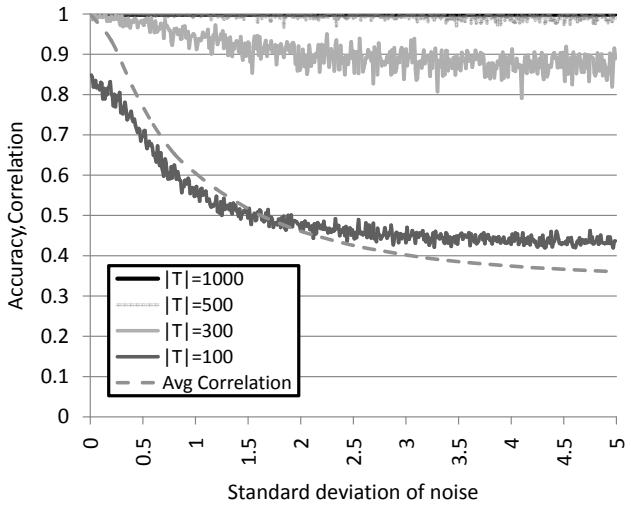


Figure 11.6: Independence experiment. Accuracy vs database size and noise. The average correlation between dependent items for a given σ is also shown.

11.5.3 Evaluating the Independence Assumption

This experiment demonstrates the validity of the independence assumption in practice. A data set was generated with a density of 0.5 containing independent and dependent itemsets. Probabilities for both were generated by the same uniform distribution between 0 and 1. In order to generate dependent itemsets of size k, additive Gaussian noise was added while "copying" an item's probabilities k times. Equal numbers of dependent and independent itemsets were generated. To evaluate the accuracy, the incremental mining algorithm was used: the number of dependent itemsets that were returned by the algorithm in the first j itemsets was calculated,

where j is the number of dependent itemsets created. The results in figures 11.5 and 11.6 clearly show that, provided the number of transactions is not too low, a very high accuracy is achieved even when the standard deviation of the noise is increased substantially. That is, as expected, the methods presented find the itemsets that are dependent, even though it was assumed that they were independent in the significance calculations. This result validates the independence assumption made in part IV of this thesis.

11.6 Conclusion

Prior to the work in chapter 10, existing methods dealing with frequent itemsets in uncertain transaction databases mine *expected* frequent itemsets, which is shown in this chapter to be inadequate as it returns itemsets that may be infrequent with high probability. This chapter introduced and solved the significant frequent itemset mining problem. Both parametric (approximate) and non-parametric (exact) tests were proposed. An extensive experimental section evaluated these methods. Furthermore, the effect of the independence assumption was evaluated and it was shown that dependent itemsets are mined with high accuracy, despite the independence assumption, thus validating this assumption for itemset mining in uncertain databases.

Chapter 12

Probabilistic Pattern Growth for Itemset Mining in Uncertain Databases

Uncertain transaction databases (UTDBs) consist of sets of existentially uncertain items. The uncertainty of items in transactions makes traditional frequent itemset mining techniques inapplicable. This chapter tackles the Probabilistic Frequent Itemset Mining (PFIM) problem, where all Probabilistic Frequent Itemsets (PFIs) are mined efficiently.
In this context, this chapter makes the following contributions: The first probabilistic FP-Growth (ProFP-Growth) algorithm and associated probabilistic FP-Tree (ProFP-Tree) are proposed. It is used to mine all probabilistic frequent itemsets in uncertain transaction databases without candidate generation, resulting in a faster algorithm than the previous state of the art algorithm proposed in chapter 10. In addition, this chapter proposes an efficient technique to compute the support probability distribution of an itemset using the concept of generating functions. This is an alternative, and more intuitive approach to the method proposed in chapter 10. An extensive experimental section evaluates the impact of the proposed techniques and shows that the ProFP-Growth approach is much faster than the Apriori based algorithm.

12.1 Introduction

Mining probabilistic frequent itemsets is a recent and challenging problem [18]. Recall that in an uncertain transaction database, the information captured in transactions is *uncertain* as the existence of an item is associated with a likelihood measure or existential probability. An example of a small uncertain transaction database is given in figure 12.1. This data set will be used as a running example in this chapter.

Recall from section 10.1 that given an uncertain transaction database, it is generally not possible to determine whether an item or itemset is frequent because it is not certain whether or not it appears in transactions. In a traditional (certain) transaction database on the other hand, an algorithm can simply perform a database scan and count the transactions that include the itemset. Since this approach does not work in an uncertain transaction database, traditional frequent itemset mining methods cannot be applied to uncertain databases.

Prior to [18] (on which chapter 10 is based), expected support was used to deal with uncertain databases [25, 26, 58]. It was shown in chapters 10 and 11 that the use of expected support in probabilistic databases has significant drawbacks that can lead to misleading and even incorrect results. The proposed alternative was based on computing the entire probability distribution of itemsets' support and mining probabilistic frequent itemsets – itemsets where the probability of being frequent is high. In chapter 10, this was achieved this in linear time by employing the Poisson binomial recurrence relation. Chapter 10 adopted an Apriori-like approach to the PFIM problem, which was based on an *anti-monotone* Apriori property[1] [11] and candidate generation. However, it is well known that Apriori-like algorithms suffer a number of disadvantages. First, all candidates generated must fit into main memory and the number of candidates can become prohibitively large. Secondly, checking whether a candidate is a subset of a transaction is non-trivial. Finally, the entire database needs to be scanned multiple times. In uncertain databases, the effective transaction width is typically larger than in a certain transaction database which in turn can increase the number of candidates generated as well as the resulting space and time costs.

In certain transaction databases, the FP-Growth algorithm [47, 48] has become the established alternative. By building an FP-Tree – effectively a compressed and highly indexed structure storing the information in the database – candidate generation and multiple database scans can be avoided. However, extending this idea to mine probabilistic frequent patterns in uncertain transaction databases is non-trivial. It

[1] If if an itemset X is not frequent, then any itemset $X \cup Y$ is not frequent.

Id	Transaction
t_1	$\{A : 1.0, B : 0.2, C : 0.5\}$
t_2	$\{A : 0.1, D : 1.0\}$
t_3	$\{A : 1.0, B : 1.0, C : 1.0, D : 0.4\}$
t_4	$\{A : 1.0, B : 1.0, D : 0.5\}$
t_5	$\{B : 0.1, C : 1.0\}$
t_6	$\{C : 0.1, D : 0.5\}$
t_7	$\{A : 1.0, B : 1.0, C : 1.0\}$
t_8	$\{A : 0.5, B : 1.0\}$

Figure 12.1: An uncertain transaction database that will be used as a running example. The set of items is $I = \{A, B, C, D\}$. Each item is associated with its probability of existing in a transaction. Items with an existence probability of 0 are not recorded. In this database, the probability that the world exists in which t_1 contains items A and C and t_2 contains only item D (and all other transactions are ignored for simplicity) is $P(A \in t_1) * (1 - P(B \in t_1)) * P(C \in t_1) * (1 - P(A \in t_2) * P(D \in t_2) = 1.0 \cdot 0.8 \cdot 0.5 \cdot 0.9 \cdot 1.0 = 0.36$.

should be noted that all previous extensions of FP-Growth to uncertain databases used the expected support approach [7, 57], which is much easier to adapt to FP-Growth since it is based on a single value, not an entire probability distribution.

This chapter proposes a compact data structure called the probabilistic frequent pattern tree (*ProFP-tree*) which compresses probabilistic databases and allows the efficient extraction of the existence probabilities required to compute the support probability distribution and frequentness probability. Additionally, this chapter proposes the novel *ProFP-Growth* algorithm for mining all probabilistic frequent itemsets without candidate generation.

12.1.1 Problem Definition and Data Model

This chapter solves the Probabilistic Frequent Itemset Mining (PFIM) problem (definition 10). Like chapter 10, it focuses on the two distinct problems of efficiently calculating the support probability distribution (definition 10.8) and efficiently extracting all probabilistic frequent itemsets (PFIs) (definition 10.4).

The uncertain data model applied in this chapter is based on the possible worlds semantic with existential uncertain items as introduced in chapter 10. If necessary, the reader may like to refer back to section 10.1.1 for an explanation and the required definitions. Also, recall that a summary of the notation was provided in figure 10.3.

As with chapters 10 and 11 it is assumed that uncertain transactions are mutually independent, and items within transactions are mutually independent. Recall this

was justified theoretically in chapters 10 and 11 and experimentally in chapter 11.

12.1.2 Contributions

This chapter makes the following contributions:

- It introduces the *Probabilistic Frequent Pattern Tree* (*ProFP-Tree*) and shows how it is built efficiently. This is the first FP-Tree type approach for handling uncertain or probabilistic data. This tree efficiently stores a probabilistic database and enables efficient extraction of itemset occurrence probabilities and database projections (conditional ProFP-Trees).
- It proposes *ProFP-Growth*, an algorithm based on the *ProFP-Tree* which mines all PFIs without using expensive candidate generation.
- It presents an intuitive and efficient method for computing the frequentness probability, as well as the entire support probability distribution, in $O(|T| \cdot minSup)$ time. This has the same time complexity as the approach based on Poisson binomial recurrence / dynamic programming technique in chapter 10, but it is more intuitive and thus offers advantages.

12.1.3 Organisation

The remainder of this chapter is organized as follows; section 12.2 surveys related work. Section 12.3 presents the ProFP-Tree, explains how it is constructed and briefly introduces the concept of conditional ProFP-Trees. Section 12.4 describes how probability information is extracted from a (conditional) ProFP-Tree. Section 12.5 introduces the generating function approach for computing the frequentness probability and the support probability distribution in linear time. Section 12.6 describes how conditional ProFP-Trees are built. Finally, section 12.7 describes the ProFP-Growth algorithm by drawing together the previous sections. The experimental evaluation is presented in section 12.8 and this chapter concludes in section 12.9.

12.2 Related Work

Recall that section 10.2 provided an in depth discussion of work related to frequent itemset mining in uncertain and probabilistic databases. This also applies to the work in this chapter.

Prior to the work in this chapter, state-of-the-art (and only) approach for probabilistic frequent itemset mining (PFIM) in uncertain databases was proposed in chapter 10 (and the associated publication [18]). That approach used an Apriori-like algorithm to mine all probabilistic frequent itemsets and the Poisson binomial recurrence to compute the support probability distribution function (SPDF). This chapter provides a faster solution by proposing the first probabilistic frequent pattern growth approach (ProFP-Growth), thus avoiding expensive candidate generation and allowing PFIM to be performed in large databases. Furthermore, a more intuitive generating function method is proposed in order to compute the SPDF.

Previous methods extending FP-Growth [47] to uncertain databases (such as the UF-Growth algorithm in [58]) use the expected support method, which is much simpler to apply but has significant disadvantages which were outlined in chapters 10 and 11.

FP-Growth is based on the idea of generating a compact in memory tree structure that captures the support information of the entire database. When this tree – the FP-Tree – fits in memory, the candidate generation and multiple database passes of the Apriori method are avoided. Furthermore, the FP-Growth algorithm avoids the subset-checking that makes Apriori sensitive to databases with a wide transaction width. A good introduction to the FP-Growth method can be found in [88].

12.3 Probabilistic Frequent-Pattern Tree (ProFP-Tree)

This section introduces a novel prefix-tree structure that enables fast detection of probabilistic frequent itemsets without the costly candidate generation or multiple database scans that plague Apriori style algorithms. By itself, it functions as an efficient compressed data structure that allows the fast retrieval of all item probabilities. The proposed structure is based on the frequent-pattern tree (FP-Tree [47]). In contrast to the FP-tree, the ProFP-tree has the ability to compress uncertain and probabilistic transactions. If a data set contains no uncertainty it reduces to the (certain) FP-Tree.

Definition 12.1. A Probabilistic Frequent Pattern Tree (ProFP-Tree) is composed of the following three components:

1. ***Uncertain item prefix tree***: A root labeled "null" pointing to a set of prefix trees each associated with uncertain item sequences. Each node n in a prefix tree is associated with an (uncertain) item a_i and consists of five fields:

- $n.item$ denotes the item label of the node. Let $path(n)$ be the set of items on the path from $root$ to n.
  - $n.count$ is the number of *certain* occurrences of $path(n)$ in the database.
  - $n.uft$, denoting "uncertain-from-this", is a set of transaction ids ($tids$). A tid for transaction t is contained in uft if and only if $n.item$ is uncertain in t (i.e. $0 < P(n.item \in t) < 1$) and $P(path(n) \subseteq t) > 0$.
  - $n.ufp$, denoting "uncertain-from-prefix", is a set of transaction ids. A tid for transaction t is contained in ufp if and only if $n.item$ is certain in t ($P(n.item \in t) = 1$) and $0 < P(path(n) \subseteq t) < 1$.
  - $n.nodeLink$ links to the next node in the tree with the same $item$ label if there exists one. Otherwise $nodeLink$ is null.

2. ***Item header table***: This table maps all items to the first node in the *Uncertain item prefix tree* with the same item label.

3. ***Uncertain-item look-up table***: This table maps ($item$, tid) pairs to the probability that $item$ appears in t_{tid} for each transaction t_{tid} contained in a uft of a node n with $n.item = item$.

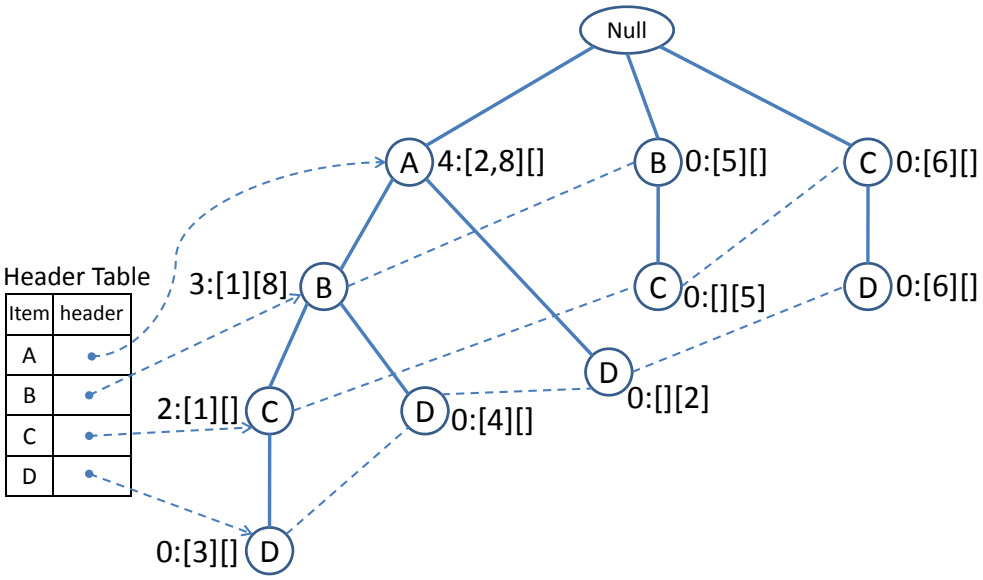
The two sets, uft and ufp, are specialized fields required in order to handle the existential uncertainty of itemsets in transactions associated with $path(n)$. These two sets are required in order to distinguish where the uncertainty of an itemset (path) comes from. Generally speaking, the entries in $n.uft$ are used to keep track of existential uncertainties where the uncertainty is caused by $n.item$, while the entries in ufp keep track of uncertainties of itemsets caused by items in $path(n) - n.item$ but where $n.item$ is certain.

Figure 12.2 illustrates the ProFP-tree of the example database of figure 12.1. Each node of the *uncertain item prefix tree* is labeled by the field $item$. The labels next to the nodes refer to the node fields in the following notation: $count : uft\, ufp$. The dotted lines denote the $nodeLinks$.

The ProFP-tree has similar advantages of a FP-tree, in particular;

1. It avoids repeatedly scanning the database since the uncertain item information is efficiently stored in a compact structure.

2. Multiple transactions sharing identical prefixes can be merged into one, where the number of certain occurrences are registered by $count$ and the uncertain occurrences reflected in the transaction sets uft and ufp. Note however that this merging is more complicated in the probabilistic ProFP-Tree.



(a) *Uncertain item prefix tree* with *item header table*. The labels next to the nodes refer to the node fields in the following notation: $count : uft\,ufp$.

$(1, B) \rightarrow 0.2$	$(1, C) \rightarrow 0.5$	$(2, A) \rightarrow 0.1$
$(3, D) \rightarrow 0.4$	$(4, D) \rightarrow 0.5$	$(5, B) \rightarrow 0.1$
$(6, C) \rightarrow 0.1$	$(6, D) \rightarrow 0.5$	$(8, A) \rightarrow 0.5$

(b) Uncertain-item lookup table. This figure simply lists the entries that would be stored in a map or hashtable.

Figure 12.2: *ProFP-Tree* generated from the uncertain transaction database given in figure 12.1.

12.3.1 ProFP-Tree Construction

The ProFP-Tree can be constructed from an UTDB T as defined by algorithm 12.1 as follows: After initializing the components of the ProFP-Tree, that is, the *uncertain item prefix tree*, *item header table* (*iht*) and the *uncertain-item look-up table* (*ult*), the tree is constructed by sequentially adding the transactions in T. Assume that the (uncertain) items in the transactions are lexicographically ordered (an ordering is required for prefix tree construction). The transactions are added to the tree in `insert-transaction()`. This method starts at the root of the tree and traverses it, following an existing path as long as the prefix of the current transaction t_i matches with that already present. When the transactions prefix no longer matches, a new branch of the tree is created to represent the remainder of the transaction (its suffix). During this traversal, the items and their probabilities are registered at the nodes visited by calling the `update-node-entries()`. This method increments the *count*

of a node if the current item and all preceding items are certain in t_i. If the current item is certain but one of its preceding items not, then t_i is registered in ufp. If the current item is uncertain, then t_i is registered in uft. This insertion process is repeated until all transactions are added to the tree.

12.3.1.1 Example

For further illustration, refer to the example database of figure 12.1 and the corresponding ProFP-tree in figure 12.2.

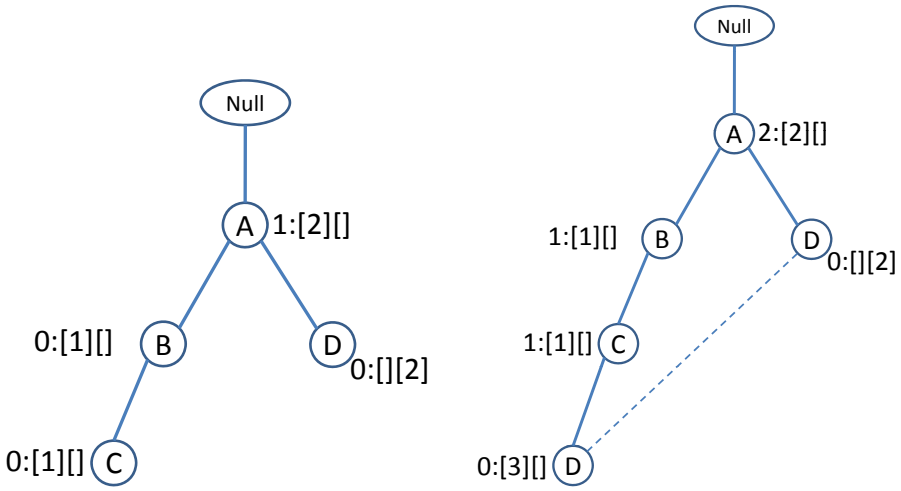
The algorithm first creates the root of the uncertain item prefix tree labeled "*null*". It then reads the uncertain transactions one at a time. While scanning the first transaction t_1, the first branch of the tree can be generated leading to the first path composed of entries of the form $(item, count, uft, ufp, node-link)$. In the example, the first branch of the tree is built by the following path:

$$\langle root, (A, 1, [], [], null), (B, 0, [1], [], null), (C, 0, [1], [], null)\rangle$$

Note that the entry "1" in the field *uft* of the nodes associated with B and C indicate that item B and C are existentially uncertain in t_1. Next, the second transaction (t_2) is scanned and the tree structure is updated accordingly. Since t_2 shares a prefix with t_1, the algorithm follows the existing path in the tree starting at the root and updates this path. Since the first item A in t_2 is existentially uncertain – that is, it exists in t_2 with a probability of 0.1 – *the count* of the first node in the path is not incremented. Instead, t_2 is added to *uft* of this node. The next item D in t_2 does not match the next node on the existing path and thus a new branch leading to a new leaf node n with entry $(D, 0, [], [2], null)$ is added. Although item D is existentially certain in t_2, the *count* of n is initialized with zero because n represents the set $\{A, D\}$ and this path from the root to node n is existentially uncertain in t_2 due to the existential uncertainty of item A. Hence, transaction t_2 is counted in the *uncertain-from-prefix (ufp)* field of n. This results in the ProFP-Tree illustrated in figure 12.3(a).

The next transaction to be scanned is t_3. Again, due to matching prefixes the algorithm follows the already existing path $\langle A, B, C\rangle$[2] while scanning the (uncertain) items in t_3. The resulting tree is illustrated in figure 12.3(b). Since the first item A exists for certain, *count* of the first node in the prefix path is incremented by one.

[2]To simplify matters, the *item* fields are used to address the nodes in a path. That is, the values of the nodes are omitted.



(a) After inserting t_1 and t_2 (b) After inserting t_1, t_2 and t_3

Figure 12.3: *Uncertain item prefix tree* after insertion of the first transactions.

The next items, B and C, are registered in the tree in the same way by incrementing the *count* fields. The rational for these *count* increments is that the corresponding prefix itemsets are certain in t_3. That is, $\{A\}$, $\{A, B\}$ and $\{A, B, C\}$ are certain itemsets in t_3. The final item D is processed by adding a new branch below the node C and leading to a new leaf node with the fields: $(D, 0, [3], [], ptr)$, where the link ptr points to the next node in the tree labeled with D. Since D is uncertain in t_3 the *count* field is initialized with 0 and t_3 is registered in the uft set: $uft = [3]$.

The *uncertain item prefix tree* is completed by scanning all remaining transactions in a similar fashion. Whenever a new node is created where the *item* does not occur anywhere else in the tree, a new entry (*item*, *ptr*) is created in the *item header table* where the link *ptr* points to the new node. Furthermore, for each new entry *tid* in a uft set of a node, a new entry $(tid, item, p)$ is added in the *uncertain-item look-up table*, where p denotes the probability that *item* exists in transaction t_{tid}. The final ProFP-tree when all transactions are added is shown in figure 12.2.

12.3.2 Complexity

The construction of the ProFP-tree requires a single scan of the uncertain transaction database T. The processing of a transaction requires the algorithm to traverse and update or construct a single path of the ProFP-Tree. This path has length equal to the number of items in the corresponding transaction, and each of the updates is completed in constant time. Therefore the ProFP-tree is constructed in linear time

Algorithm 12.1 ProFP-Tree Construction algorithm. Note that it is not hard to add an additional scan whereby the items are sorted in decreasing order by their frequentness probability and only those items that are probabilistic frequent are used to build the tree, analogous to the sorting of items by support in the (certain) FP-Growth algorithm.

```
Input: An uncertain transaction Database T with
 lexicographically ordered items, and a minimum
 support threshold minSup.

Output: A probabilistic frequent pattern tree (ProFP-Tree).

Method:
 Create the (null) root of an uncertain item prefix tree tree;
 Initialize an empty item header table (iht);
 Initialize an empty uncertain-item look-up table (ult);
 for each uncertain transaction t_i ∈ T
  assume t_i is a string <it_1,···,it_n> of tuples it_j=(item,prob),
  where the field item identifies a(n) (un)certain item of t_i
  and the field prob denotes the probability P(it_j.item ∈ t_i).
  Call insert-transaction(<it_1,···,it_n>,i,tree.root,0)

insert-transaction(transaction,i,node,u_flag)
 for each it ∈transaction
  if node has a child n with n.item = it.item
   //follow an existing path
   call update-node-entries(it,i,n,u_flag);
  else //create a new path:
   create new child n of tree;
   call update-node-entries(it,i,n,u_flag);
   if it.item not in iht
    insert (it.item,n) into iht;
   else
    insert n into the node list associated with it.item;
  //update uncertain item lookup table
  if it.prob < 1.0
   insert (i,it.item,it.prob) into ult;
  node = N;

update-node-entries(it,i,n,u_flag)
  if it.prob = 1.0
   if u_flag = 0
    increment n.count by 1;
   else
    insert i into n.ufp;
  else
   insert i into n.uft;
   u_flag = 1;
```

with respect to the size of the database – $O(|T| \cdot |I|)$ where $|T|$ is the number of transactions and $|I|$ is the number of items.

Since the ProFP-Tree is based on the original FP-Tree (that is, the prefix-tree part has the same structure), it inherits its compactness properties. In particular, the size of a ProFP-Tree is bounded by the overall occurrences of the items in the database and its height is bounded by the maximal number of items in a transaction.

For any transaction t_i in T, there exists exactly one path in the ProFP-Tree starting below the *root* node. Each item within a transaction in the transaction database can create no more than one node in the tree and the height of the tree is bounded by the number of items in a transaction (path). Note that as with the FP-Tree, the compression is obtained by sharing common prefixes.

It is now shown that the values stored at the nodes do not affect the bound on the size of the tree. In particular, the following lemma bounds the *uncertain-from-this* (uft) and *uncertain-from-prefix* (ufp) sets. Note that *count* and *nodeLink* have constant size.

Lemma 12.2. *Let tree be the* ProFP-Tree *generated from an uncertain transaction database T. The total space required by all the transaction-id sets (*uft *and* ufp*) in all nodes in tree is bounded by the the total number of entries in transactions with an existential probability in* $(0, 1)$*. That is, the number of probabilities in* $(0, 1)$ *in* T*.*

Proof. Each occurrence of an uncertain item (with existence probability in $(0, 1)$) in the database yields at most one transaction-id entry in one of the transaction-id sets assigned to a node in the tree. In general there are three update possibilities for a node n: If the current item and all prefix items in the current transaction t_i are certain, there is no new entry in uft or ufp as *count* is incremented. t_i is registered in $n.uft$ if and only if $n.item$ is existentially uncertain in t_i while t_i is registered in $n.ufp$ if and only if $n.item$ is existentially certain in in t_i but at least one of the prefix items in t_i is existentially uncertain. Therefore each occurrence of an item in T leads to either a count increment (which does not require additional space) or one new entry in uft or ufp. □

Finally, it should be clear that the size of the *uncertain item look-up table* is bounded by the number of uncertain (non zero and non 1) entries in the database.

This section showed that the ProFP-Tree inherits the compactness of the original FP-tree. The next section shows that the information stored in the ProFP-Tree suffices to retrieve all probabilistic information required for PFIM, thus proving completeness.

12.4 Extracting Certain and Uncertain Support Probabilities

Unlike the (certain) FP-Growth approach where it is easy to extract the support of an itemset X by summing the support counts along the node-links for X in a suitable conditional ProFP-Tree, this chapter is concerned with the support distribution of X in the probabilistic case. Before this can be computed however, both the number of certain occurrences as well as the probabilities $0 < P(X \in t_i) < 1$ are required. Both can be efficiently obtained using the ProFP-Tree as follows:

- To obtain the *certain* support of an item x, the algorithm follows the node-links from the *item header table* and accumulates both the counts and the number of transactions in which x is *uncertain-from-prefix*. The latter is counted since the support of x is required and by construction, transactions in ufp are known to be certain for x (but uncertain from the prefix).
- To find the set of transaction ids in which x is uncertain, the algorithm follows the node-links as above and accumulate all transactions that are in the uncertain-from-this (uft) list.

Example 12.3. Consider item C in the ProFP-Tree of figure 12.2. By traversing the node-list for C, we can reach three nodes which are accumulated as follows in order to calculate the certain support: $(2 + |\emptyset|) + (0 + |\{t_5\}|) + (0 + |\emptyset|) = 3$. Note there is one transaction in which C is *uncertain-from-prefix* (t_5). Similarly, in this same traversal it is easy to obtain the transaction ids for the transactions in which C is uncertain: $[1] \cup \emptyset \cup [6] = [1, 6]$. That is, the only transactions in which C is uncertain are t_1 and t_6. The exact appearance probabilities in these transactions can be obtained from the *uncertain-item look-up table* (figure 12.2(b)): the probabilities of C appearing in transactions t_1 and t_6 are 0.5 and 0.4, respectively. By comparing these results to the original database in figure 12.1), it is easy to see that the tree allows the certain support as well as the transaction ids where C is uncertain to be found efficiently.

To compute the support of an itemset $X = \{B, C, D, ..., K\}$, the conditional tree for $\{C, D, ..., K\}$ is required, from which the certain support and uncertain transaction ids for the nodes labeled B can be obtained. These implicitly correspond to the entire itemset X. Since it is somewhat involved, the construction of conditional ProFP-Trees is deferred to section 12.6. For now it suffices to state that by using

Algorithm 12.2 Algorithm to extract the probabilities for an item, or the probabilities for an itemset if *tree* is a conditional ProFP-Tree.

```
//calculate the certain support and the uncertain
//transaction ids of an item derived from a ProFP-Tree
extract(item, ProFPTree tree)
 certSup = 0; uncertainSupTids = ∅;
 for each ProFPNode in tree reachable
 from header table[item]
  certSupp+ = n.certSupp;
  certSupp+ = |n.ufp|;
  uncertainSupTids = uncertainSupTids ∪ n.uft;
 return certSupp, uncertainSupTids;

//calculate the existential probabilities of an itemset
calculateProbabilities(itemset, uncertainSupTids)
 probabilityVector = ∅;
 for (t ∈ uncertainSupTids)
  p = Π_{i in itemset} uncertainItemLookupTable[i, t];
  probabilityVector.add(p);
 return probabilityVector;
```

the conditional tree, the above method provides the certain support of X ($certSup$) and the exact set of transaction ids in which X is uncertain ($utids$). To compute the probabilities $P(X \in t_i) : t_i \in utids$ where $utids$ are the transaction ids in which $0 < P(X \in t_i) < 1$, the independence assumption is used: $P(X \subseteq t_i) = \Pi_{x \in X} P(x \in t_i)$.

Recall that $P(x \in t_i)$ is an $O(1)$ look-up in the *uncertain-item look-up table*.

It has now been described how the certain support and all probabilities $P(X \in t) : X\, uncertain\, in\, t$ can be efficiently computed from the ProFP-Tree. Algorithm 12.2 shows the concrete algorithm for performing this task. Section 12.5 describes how this information is used to to efficiently calculate the support distribution and frequentness probability of X.

12.5 Efficient Computation of Probabilistic Frequent Itemsets

This section presents a technique to compute the probabilistic support (the *support probability distribution*) of an itemset using generating functions. The problem can be defined as follows:

Definition 12.4. Given a set of N mutually independent but in general *non-identical* Bernoulli random variables $P(X \in t_i)$, $1 \leq i \leq N$, compute the probability distribution of the random variable $Sup = \sum_N^{i=1} X_i$.

Note that N is the number of transactions, $|T|$. A naive solution is to count all possible worlds in which exactly k transactions contain X and accumulate the respective probabilities for every possible support value k: $0 \leq k \leq N$. This approach has a complexity of $O(2^N)$ due to the enumeration of the possible worlds. Chapter 10 proposed an approach that achieves a $O(N \cdot minSup)$ complexity using the Poisson binomial recurrence. This work proposes a different approach that, albeit having the same asymptotic complexity, has other advantages.

12.5.1 Efficient Computation of Probabilistic Support

This chapter applies the concept of generating functions as proposed in the context of probabilistic ranking in [59]. Consider the function: $\mathcal{F}(x) = \prod_{i=1}^{n}(a_i + b_i x)$. The coefficient of x^k in $\mathcal{F}(x)$ is given by:

$$\sum_{\beta:|\beta|=k} \prod_{i:\beta_i=0} a_i \prod_{i:\beta_i=1} b_i$$

where $\beta = \langle \beta_1, ..., \beta_N \rangle$ is a boolean vector and $|\beta|$ denotes the number of 1's in β. Note that the sum is over all possible β and therefore covers all possible combinations in which x has a power of k.

Consider the following generating function:

$$\mathcal{F}^j(x) = \prod_{t \in \{t_1, t_2, ..., t_j\}} (1 - P(X \in t) + P(X \in t) \cdot x) = \sum_{i \in \{0,...,j\}} c_{i,j} x^i.$$

The coefficient $c_{i,j}$ of x^i in the expansion of $\mathcal{F}^j(x)$ is the probability that X occurs in exactly i of the first j transactions; that is, $P_{ij}(X)$ (recall the notation from figure 10.3). Note therefore that the probability that X occurs in at least i of the first j transactions is $P_{\geq i,j} = \sum_{k \geq i} c_{k,j}$, and the frequentness probability can be calculated as $P_{\geq minSup} = \sum_{k \geq i} c_{k,N}$ where the $c_{k,N}$ are taken from $\mathcal{F}^N(x)$.

Since $\mathcal{F}^j(x)$ contains at most $j + 1$ nonzero terms and by observing that

$$\mathcal{F}^j(x) = \mathcal{F}^{j-1}(x) \cdot (1 - P(X \in t_j) + P(X \in t_j) \cdot x)$$

it follows that $\mathcal{F}^j(x)$ can be computed in $O(j)$ time given $\mathcal{F}^{j-1}(x)$ (this is the time taken to expand the terms). Since $\mathcal{F}^0(x) = 1x^0 = 1$ is the starting point (this is the probability that an itemset occurs 0 times in the first 0 transactions), $\mathcal{F}^N(x)$ can be computed in $O(N^2)$ time. This run time complexity can be reduced by exploiting the fact that only the coefficients c_i where $i < minSup$ need to be considered in $\mathcal{F}^N(x)$. The reasons for this are as follows: The frequentness probability of X is defined as

$$P(X\,is\,frequent) = P_{\geq minSup}(X) = P(Sup(X) \geq minSup))$$

$$= 1 - P(Sup(X) < minSup) = 1 - \sum_{i=0}^{minSup-1} c_i$$

and a coefficient $c_{i,j}$ in $\mathcal{F}^j(x)$ is independent of any $c_{k,j-1}$ in $\mathcal{F}^{j-1}(x)$ where $k > i$. That means in particular that the coefficients $c_{k,j}$, $k \geq minSup$ are not required to compute the $c_{i,j}$, $i < minSup$.

Thus, considering only the coefficients $c_{i,j}$ where $i < minSup$, $\mathcal{F}^j(x)$ contains at most $minSup$ coefficients that need to be evaluated, leading to a total complexity of $O(minSup \cdot N)$. Recall that $N = |T|$ and that this is the same complexity as the method based on the Poisson binomial recurrence of chapter 10.

Example 12.5. Consider itemset $\{A, B\}$ in the example database of figure 12.1. Recall that using a conditional *ProFP-Tree*, it is easy and efficient to extract, for each transaction t_i, the probability $P(\{A, B\} \in t_i)$ where $0 < P(\{A, B\} \in t_i) < 1$ as well as the number of certain occurrences of $\{A, B\}$. Itemset $\{A, B\}$ occurs for certain only in t_4 and occurs in t_1, t_2 and t_3 with a probability of 0.2, 0.1, and 0.3 respectively. Let $minSup$ be 2. Then:

$$\mathcal{F}^1(x) = \mathcal{F}^0(x) \cdot (0.8 + 0.2x) = 0.2x^1 + 0.8x^0$$

$$\mathcal{F}^2(x) = \mathcal{F}^1(x) \cdot (0.9 + 0.1x) = ... + 0.26x^1 + 0.72x^0$$

$$\mathcal{F}^3(x) = \mathcal{F}^2(x) \cdot (0.7 + 0.3x) = ... + 0.418x^1 + 0.504x^0$$

Thus, $P(sup(\{A, B\}) = 0) = 0.504$ and $P(sup(\{A, B\}) = 1) = 0.418$. Consequently, $P(sup(\{A, B\}) \geq 2) = 0.078$ $(1 - 0.504 - 0.418)$. Thus, A, B is not returned as a frequent itemset if τ is greater than 0.078. Indeed, it is very unlikely that $\{A, B\}$ is frequent. In the above Equations, note that only the c_i where $i < minSup$ needed to be computed.

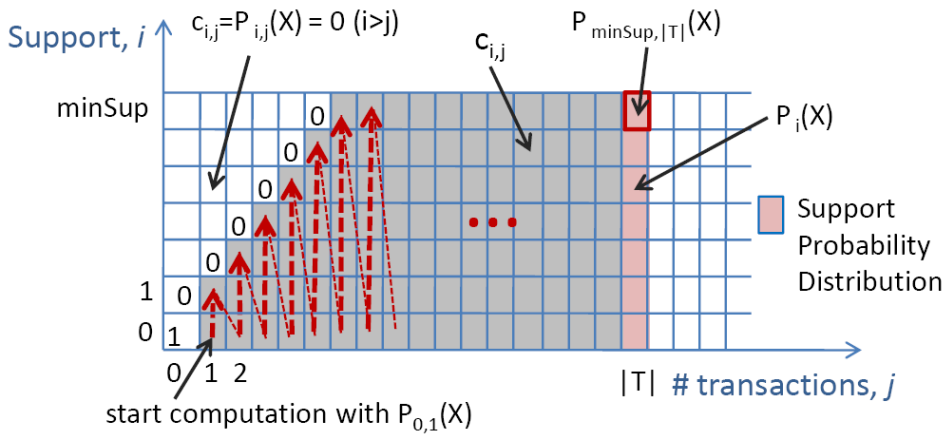


Figure 12.4: Visualisation of the frequentness probability computation using the generating function coefficient method.

This approach can be visualised using the matrix in figure 12.4. Each cell $c_{i,j} = P_{i,j}(X)$ and therefore the matrix contains the entire probability distribution of the support of X. The jth column contains the coefficients of $\mathcal{F}^j(x)$. Hence, the computation progresses by calculating the columns one at a time, as shown in the figure. Note that the frequentness probability $P_{\geq minSup,|T|}(X)$ can be calculated by subtracting the column sum from 1, as the jth column sum is the probability that X has support less than $minSup$ in the first j transactions. In contrast, recall that the computation matrix for the Poisson binomial computation method in chapter 10 has cells with $P_{\geq i,j}(X)$ and computed one row at a time.

In order to compute each successive column, only the previous column is needed, hence the space required is $O(minSup)$. Note that this is less than the $O(|T|)$ space required by the Poisson binomial method.

12.5.1.1 Pruning using a Lower Bound

Note that after the calculation of the first $minSup$ coefficients of each $\mathcal{F}^j(x)$, it is possible to stop the computation when $P_{minSup,j}(X) = 1 - \sum_{i<minSup} c_{i,j} \geq \tau$ since this means that the respective itemset is frequent with probability at least τ. Intuitively, if an itemset X is already a PFI considering only the first j transactions, X will still be a PFI if more transactions are considered as the frequentness probability can only increase (recall this was encoded in lemma 10.15). This pruning method can be used if the exact frequentness probability does not need to be calculated. Note that an application where this is useful is the Significant Frequent Itemset Mining (SiFIM) method of chapter 11. Recall that significant frequent itemsets can

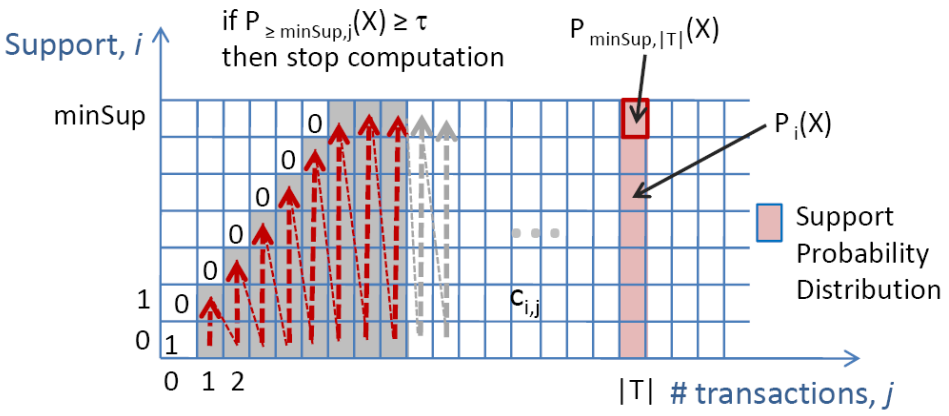


Figure 12.5: Upper bound pruning in the computation of the frequentness probability using generating functions.

be computed by adapting the frequentness probability computation. By adapting the method presented here, the computation can be stopped if it is clear that the itemset is significant. The $pValue$ is not required.

Figure 12.5 illustrates this pruning concept. Note that this pruning method is not the same as the pruning criterion proposed in chapter 10. In fact, the method used here cannot be applied in the Poisson binomial recurrence approach as it requires i to reach $minSup$. Therefore, it is suited to methods where columns are computed. In chapter 10, the calculation progressed row-wise, and therefore by the time the pruning could be employed, almost the entire matrix would have been computed already.

12.5.1.2 Pruning using an Upper Bound

A natural question to ask is whether the pruning from chapter 10 can be applied here. Recall that if $P_{\geq minSup-d,|T|-d}(X) < \tau$, $1 \leq d \leq minSup$, then the computation can be immediately pruned since it is already clear that X cannot be a PFI by lemma 10.17. This can be applied to the method above at every such cell. Note however that using this pruning method saves some columns, while in the method of chapter 10 it saves the computation of rows. Since typically $minSup << |T|$, one can expect that pruning rows is more efficient.

12.5.1.3 Certainty Optimisation

Note that the approach introduced in chapter 10 for avoiding the consideration of $P(X \in t) = 0$ or $P(X \in t) = 1$ is directly applicable here too. Recall that trans-

actions t where $P(X \in t) = 0$ can be ignored, and transactions with $P(X \in t) = 1$ can be ignored by decrementing $minSup$. Note that the first optimisation is done automatically when one used the ProFP-Tree, and the second one is made much easier with the ProFP-Tree as it stores the certain support separately.

12.5.1.4 Discussion

The generating function technique is different to the Poisson binomial recurrence method, but has the same run time complexity. This section weights up their respective benefits and downsides.

Using generating functions instead of the recursion formula gives a different and intuitive view of the problem. It can be argued that it is clearer, since the coefficients correspond to the support distribution. It also leads to a method for computing the frequentness probability in less space. The column wise computation method allows a new pruning method that cannot be applied to the recurrence method. An additional advantage of this approach is that it allows an iterative database scan in a candidate generation type method. By storing an array of length $minSup$ for each candidate, one can scan the database one transaction at a time and update all the coefficients per transaction. In one scan, all the probabilities for all candidates can be incrementally computed. As described above, itemsets can be pruned before all transactions are considered using both a lower bound and an upper bound. In contrast, the row based method does not lend itself to such a method, because probabilities in all transactions are required to compute the first – and all subsequent – rows. While this observation is not an advantage in the ProFP-Growth algorithm, it could be an advantage in ProApriori – allowing it to use less space and avoid keeping the database in memory.

In addition, the generating function approach allows the support probability density function to be updated easily if the probability that a transaction t_i contains an itemset X changes. That is, if the probability $p = P(X \in t_i)$ changes to p', then it is possible to update the support probability distribution by dividing the generating function by $px + (1 - p)$ (using polynomial division) in order to remove the effect of t_i, and subsequently, multiplying this result by $p'x + (1 - p')$ to incorporate the new probability p'. That is, $\mathcal{F}^{j\prime}(x) = \mathcal{F}^{j}(x) : (px + 1 - p) \times (p'x + 1 - p')$, where $\mathcal{F}^{j\prime}$ is the generating function for the support probability distribution of X in the first j transactions in the altered database. Note that this chapter does not consider transactions as mutable, but this possibility may be useful in some other applications.

12.6 Extracting Conditional ProFP-Trees

This section describes how conditional ProFP-Trees are constructed from other (potentially conditional) ProFP-Trees. The method for doing this is more involved than the analogous operation for the certain FP-Growth algorithm, since the information capturing the source of the uncertainty must remain correct. That is, whether the uncertainty at that node comes from the prefix or from the present node. Recall from section 12.4 that this is required in order to extract the correct probabilities from the tree. A conditional ProFP-Tree for itemset X ($tree_X$) is equivalent to a ProFP-Tree built on only those transactions in which X occurs with a non-zero probability. In order to generate a conditional ProFP-Tree for itemset $X \cup i$ ($tree_{X \cup i}$) where i occurs lexicographically prior to any item in X, first begin with the conditional ProFP-Tree for X. When $X = \emptyset$, $tree_X$ is simply the complete ProFP-Tree. $tree_{X \cup i}$ is constructed by propagating the values at the nodes for i upwards and accumulating these at the nodes closer to the root as listed in algorithm 12.3. Let N_i be the set of nodes with item label i (These are obtained by following the links from the header table). The values for every node n in $tree_{X \cup i}$ are calculated as follows:

- $n.count = \sum_{n_i \in N_i} n_i.count$ since these represent certain transactions.
- $n.uft = \cup_{n_i \in N_i} n_i.uft$ since $tree_{X \cup i}$ conditions on an item that is uncertain in these transactions and hence any node in the final conditional tree will also be uncertain for these transactions.
- When collecting transactions for n that are uncertain from the prefix (i.e. $t \in ufp$), it is necessary to determine whether the item $n.item$ caused this uncertainty. If the corresponding node in $tree_X$ contained transaction t in ufp, then t is also in $n.ufp$ ($n.item$ was not uncertain in t). If $n.item$ was uncertain in t, then the corresponding node in $tree_X$ would have t listed in uft and this must also remain the case for the conditional tree. If $t \in n.ufp$ is neither in the corresponding ufp nor uft in $tree_X$, then it must be certain for $n.item$ and $n.count$ is incremented.

12.7 ProFP-Growth Algorithm

This chapter has described four fundamental operations required for the ProFP-Growth algorithm; building the ProFP-Tree (section 12.3); efficiently extracting the certain support and uncertain transaction probabilities from it (section 12.4);

Algorithm 12.3 Construction of a conditional ProFP-Tree $tree_{X \cup i}$ by extracting item i from the conditional ProFP-Tree $tree_X$.

```
//Accumulates transactions for nodes when
//propagating up the values from a node being extracted.
class Accumulator
 count = 0; uft = ∅; ufp = ∅;
 orig_ufp = the original upf list
 add(ProFPNode n)
  count+ = n.count;
  uft = uft ∪ n.uft;
  for (t ∈ n.ufp)
   if (orig_ufp.contains(t)) ufp = ufp ∪ t;
   else if (orig_uft.contains(t)) uft = uft ∪ t;
   else count + +;

buildConditionalProFPTree(ProFPTree tree_X, item i)
  returns tree_{X∪i}
 tree_{X∪i} =clone of the sub-tree of tree_X reachable
  from header table for i;
 associate an Accumulator with each node in tree_{X∪i}
  and set orig_ufp;
 propagate(tree_{X∪i},i);
 set the certSup, uft, ufp values of nodes in tree_{X∪i}
  to those in the corresponding Accumulators;

propagate(ProFPTreetree, itemi)
 for(ProFPNode n accessible from header table for i)
  ProFPNode cn = n;
  while(cn.parent ≠ null)
   call add(n) on Accumulator for cn;
   cn = cn.parent;
```

calculating the frequentness probability and determining whether an item(set) is a probabilistic frequent itemset (section 12.5); and construction of the conditional ProFP-Trees (section 12.6). Together with the fact that probabilistic frequent itemsets possess an anti-monotonicity property, as proved in lemma 10.18 of chapter 10, it is now possible to describe the ProFP-Growth algorithm. It uses a similar approach to the certain FP-Growth algorithm and the four operations outlined in previous sections to mine all probabilistic frequent itemsets.

Like the FP-Growth algorithm, ProFP-Growth operates by extracting items and recursively building conditional ProFP-Trees for larger and larger itemsets. Algorithm 12.4 provides a listing of the ProFP-Growth algorithm.

Algorithm 12.4 Simplified ProFP-Growth algorithm. Note that if the heuristic whereby an additional database scan is used to sort items by frequentness probability, output probabilistic frequent items and remove those that are not probabilistic frequent, then the `entire if` $\alpha = \emptyset$ part of the algorithm may be omitted.

```
Input: A ProFP-Tree tree constructed based on algorithm 12.1,
 the minimum support minSup, and
 the minimum frequentness probability τ.

Output: The complete set of probabilistic frequent itemsets.

Method: call ProFPGrowth(tree,∅)

//tree is the conditional ProFP-Tree for α
ProFPGrowth(ProFP-Tree tree, Set α)
 if α = ∅
  for each item x in iht in lexicographically increasing order
   (certSupport, uncertainSupTids) = extract(x,tree)
    //Algorithm 12.2
   vector = calculateProbabilities({x},uncertainSupTids)
    //Algorithm 12.2
   calculate the support probability p
    //Section 12.5.1
   if (p ≥ τ)
    output x, p
    tree_{α∪x} =buildConditionalProFPTree(tree, x)
     //Algorithm 12.3
    ProFPGrowth(tree_{α∪x},{x})
   else
    iht.remove(x)
 else
  for each item x in iht lexicographically before elements of α
   (certSupport, uncertainSupTids) = extract(x,tree)
    //Algorithm 12.2
   vector = calculateProbabilities({x},uncertainSupTids)
    //Algorithm 12.2
   calculate the support probability p
    //Section 12.5.1
   if (p ≥ τ)
    output x, p
    tree_{α∪x} =buildConditionalProFPTree(tree, α∪{x})
     //Algorithm 12.3
    ProFPGrowth(tree_{α∪x},{x})
```

12.8 Experimental Evaluation

This section presents performance experiments on the proposed *ProFP-Growth* algorithm and compares the results to the Apriori-based solution (*ProApriori*) presented in chapter 10. In all experiments, the Poisson binomial recurrence method of chapter 10 was used in order to remove this as a variable.

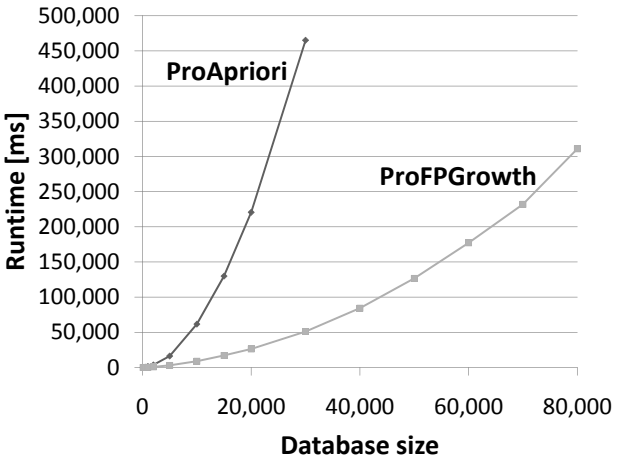
This section also analyzes how various database characteristics and parameter settings affect the performance of the ProFP-Growth algorithm. For the first set of experiments, artificial data sets were used with a variable number of transactions and items. In these databases, each item x has a probability $P_1(x)$ of appearing for certain in a transaction, and a probability $P_0(x)$ of not appearing at all in a transaction. With a probability of $1 - P_0(x) - P_1(x)$ item x is uncertain in a transaction. In this case, the probability that x exists in such a transaction is picked randomly from a uniform $(0, 1)$ distribution. For the scalability experiments[3], unless otherwise stated, the number of items and transactions were varied and $P_0(x) = 0.5$ and $P_1(x) = 0.2$ were chosen for each item. Unless otherwise stated, $minSup = 0.1 \cdot |T|$ and $\tau = 0.9$ in the run time experiments.

Additional experiments on larger well known and real databases can be found in chapter 13.

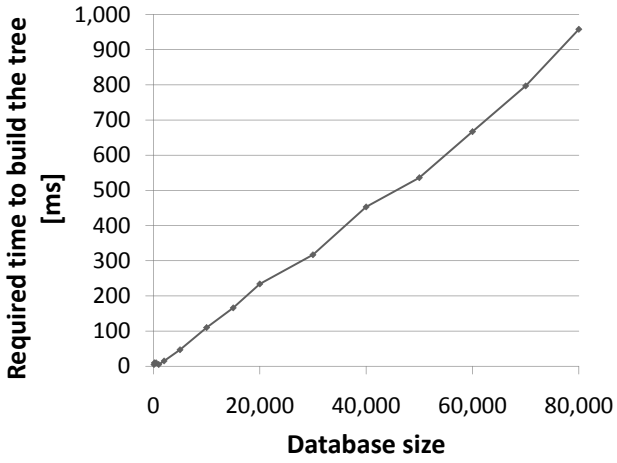
12.8.1 Number of Transactions

The number of transactions was varied and a fixed number of items (20) was used. The results can be seen in figure 12.6(a). It can be observed that *ProFP-Growth* significantly outperforms *ProApriori*. The time required to build the *ProFP-Tree* in comparison with the number of transactions is shown in figure 12.6(b). The linear time complexity indicates a constant time required to insert transactions into the tree. This is expected since the maximum height of the *ProFP-Tree* is equal to the number of items, which is constant in this experiment. Finally, the size of the *ProFP-Tree* was evaluated in this experiment as shown in figure 12.7(a). The number of nodes in the *ProFP-Tree* increases sub-linearly in comparison to the number of transactions. This occurs since new nodes are created for a transaction only if it has a suffix that is not yet contained in the tree. As the number of transactions increases, this overlap of prefixes increases, requiring fewer new nodes to be created. It can be expected that this overlap is more probable when the items' appearance are correlated with each other. Therefore, a real database was also used in this

[3] All experiments were performed on an Intel Xeon with 32 GB of RAM and a 3.0 GHz processor.



(a) Total Runtime

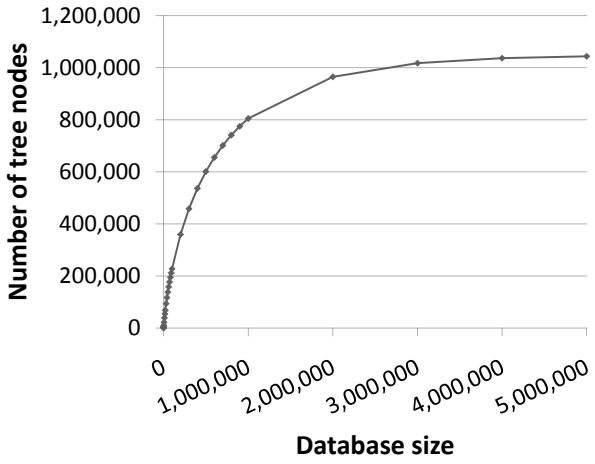


(b) Tree Generation

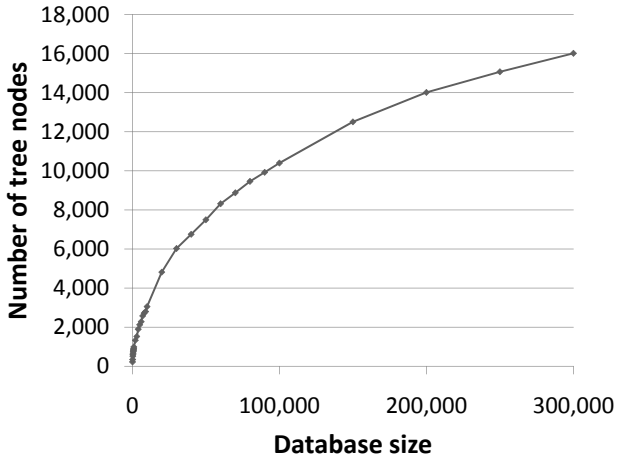
Figure 12.6: Total run time and time required to build the ProFP-Tree in comparison the the database size (number of transactions).

evaluation. The size of the *ProFP-Tree* was evaluated on subsets of the real-world data set *accidents*[4], denoted by *ACC*. It consists of 340,184 transactions and a reduced number of 20 items whose occurrences in transactions were randomized in order to obtain an uncertain database: With a probability of 0.5, each item appearing for certain in a transaction was assigned a value drawn from a uniform distribution in $(0, 1]$. This database size was varied up to the first 300,000 transactions. As can be seen in figure 12.7(b), there is more overlap between transactions since the growth in the number of nodes used is slower (compared to figure 12.7(a)).

[4]The *accidents* data set [42] was derived from the Frequent Itemset Mining Data set Repository (http://fimi.cs.helsinki.fi/data/)



(a) Tree size



(b) Tree size (*ACC*)

Figure 12.7: Tree size in comparison to database size for two databases.

12.8.2 Number of Items

Next, the number of items was varied from 5 to 100 using a fixed number of 1,000 transactions. The run times can be seen in figure 12.9(a), which shows the expected exponential run time inherent in the FIM problem. It can clearly be seen that *ProFP-Growth* outperforms *ProApriori*. In figure 12.9(b) the number of nodes of the *ProFP-Tree* is shown. Except when there are very few items, the number of nodes in the tree grows linearly. The reason for this is that the likelihood of two transactions having a common prefix of size 10 or more is low here. Hence – except for possibly the first few items – each transaction requires new nodes to be created for each item.

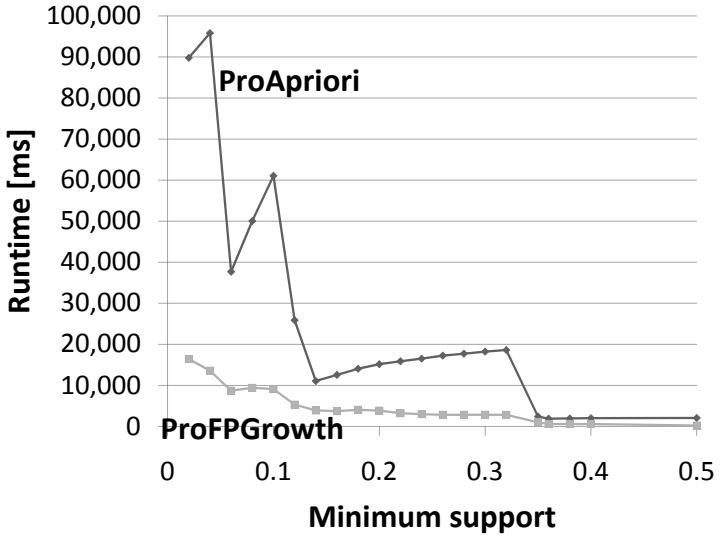


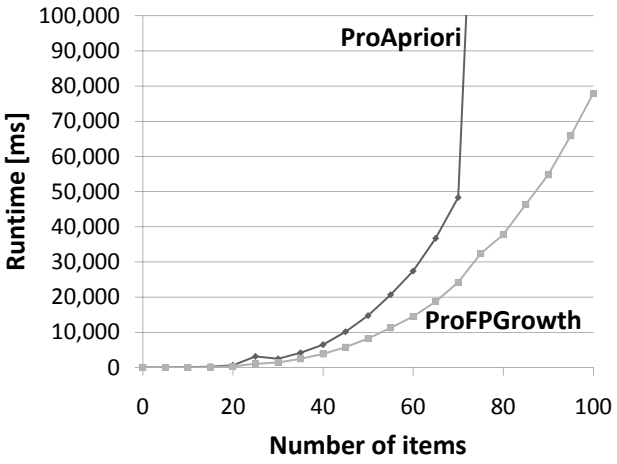
Figure 12.8: Effect of *minSup*.

12.8.3 Effect of Uncertainty and Certainty

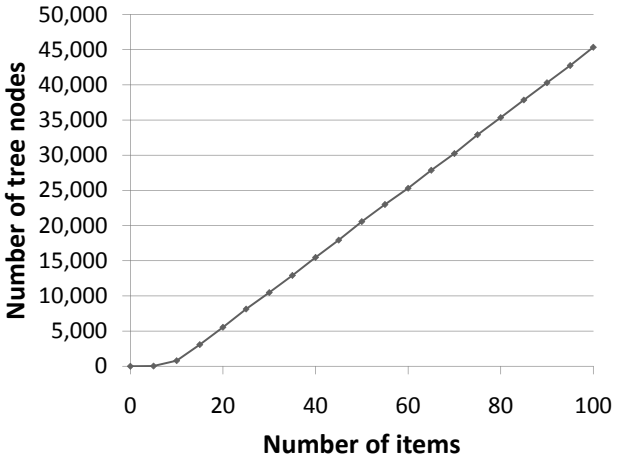
This experiment evaluates the effect of the level of certainty and uncertainty on the ProFP-Growth algorithm. The number of transactions used was 1,000, the number of items used was 20 and the parameters $P_0(x)$ and $P_1(x)$ were varied.

For the experiment shown in figure 12.10(a), the probability that items are uncertain $(1-P_0(x)-P_1(x))$ was fixed at 0.3 and $P_1(x)$ was successively increased from 0 (which means that no items exist for certain) to 0.7. The results show that the number of nodes initially increases. This is expected, since more items existing in the database increases the nodes required. However, as the number of certain items increases, an opposing effect reduces the number of nodes in the tree. This effect is caused by the increasing overlap of the transactions – in particular, the increased number and length of shared prefixes. When $P_1(x)$ reaches 0.7 (and thus $P_0(x) = 0$), each item is contained in each transaction with a probability greater than zero, and thus all transactions contain the same items with a non-zero probability. In this case, the *ProFP-Tree* degenerates to a linear list containing exactly one node for each item. Note that the size of the look-up table is constant here, since the expected number of uncertain items is constant at $0.3 \cdot |T| \cdot |I| = 0.3 \cdot 1,000 \cdot 20 = 6,000$.

In figure 12.10(b), $P_1(x)$ was fixed at 0.2 and $P_0(x)$ was successively decreased from 0.8 to 0. This increases the probability that items are uncertain from 0 to 0.8. A similar pattern in the number of nodes used emerges in the results (figure 12.10(a)). As expected in this experiment, the size of the look-up table increases as the number



(a) Runtime



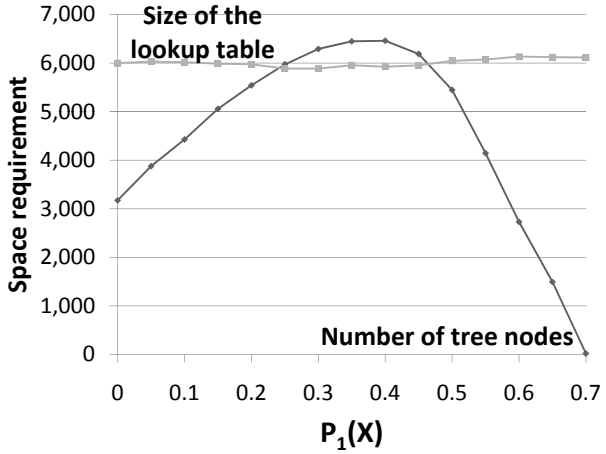
(b) Tree size

Figure 12.9: Scalability with respect to the number of items.

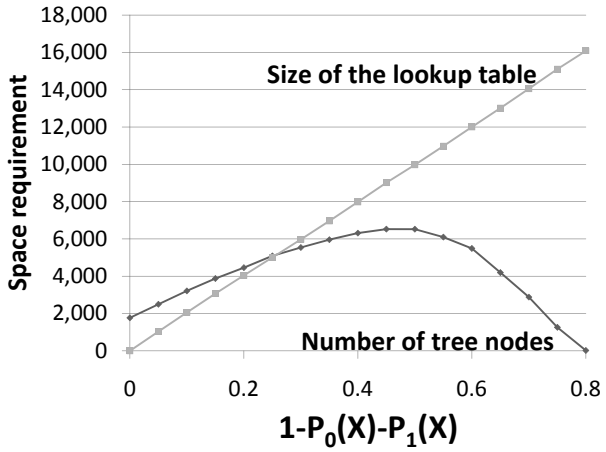
of uncertain items increases.

12.8.4 Effect of *MinSup*

Here, the minimum support threshold minSup was varied on an artificial database of 10,000 transactions and 20 items. Figure 12.8 shows the results. For low values of minSup, both algorithms have a high run time due to the large number of probabilistic frequent itemsets. It can be observed that *ProFP-Growth* significantly outperforms *ProApriori* for all settings of minSup.



(a) Varying the probability of certain occurences while keeping uncertain occurences fixed.



(b) Varying the probability of uncertain occurences while keeping certain occurences fixed.

Figure 12.10: Effect of uncertainty on the tree size

12.9 Conclusion

The Probabilistic Frequent Itemset Mining (PFIM) problem is to find itemsets in an uncertain transaction database that are (usually highly) likely to be frequent. This problem has two components; efficiently computing the support probability distribution and frequentness probability, and efficiently mining all probabilistic frequent itemsets. To solve the first problem efficiently, a novel method based on generating functions was proposed. To solve the second problem, this chapter proposed the first probabilistic frequent pattern tree (ProFP-Tree) and pattern growth algorithm (ProFP-Growth). Experiments demonstrated that this significantly outperforms the

previous state of the art ProApriori approach to PFIM (presented in chapter 10).

Chapter 13

Vectorised Probabilistic Frequent Itemset Mining using GIM

Uncertain transaction databases consist of sets of existentially uncertain items. The uncertainty of items in transactions makes traditional frequent itemset mining techniques inapplicable. This chapter tackles the Probabilistic Frequent Itemset Mining (PFIM) problem.
In this context, this chapter makes the following contributions: The first vectorised algorithm for solving the PFIM problem is proposed, resulting in a much faster algorithm than the previous state of the art algorithms proposed in chapters 10 and 12. In particular, it is shown that the PFIM problem can be solved by the Generalised Interaction Mining (GIM) framework and algorithm of chapter 3. An extensive experimental section evaluates GIM-PFIM and shows that it is orders of magnitude faster and used orders of magnitude less space than ProFP-Growth and Pro-Apriori.

13.1 Introduction

Mining probabilistic frequent itemsets is a recent and challenging problem [18]. Recall from chapter 10 that in an Uncertain Transaction Database (UTDB), the information captured in transactions is *uncertain* as the existence of an item is associated with a likelihood measure or existential probability. Figure 12.1 shows the UTDB that will be used as a running example in this chapter.

Recall from section 10.1 that given an uncertain transaction database, it is generally not possible to determine whether an item or itemset is frequent because it is not certain whether or not it appears in transactions. Consequently, traditional frequent itemset mining methods cannot be applied to UTDBs.

Prior to the work in chapters 10, 11 and 12, expected support was used to deal with uncertain databases [25, 26]. This method was shown to have significant drawbacks, causing misleading and even incorrect results. The proposed alternative is based on computing the entire support probability distribution, but doing so very efficiently. Subsequently, either *probabilistic frequent itemsets* (chapters 10 and 12) or *significant frequent itemsets* (chapter 11) were mined.

However, the algorithm in which these methods were embedded has a large impact on the run time of the overall mining algorithm. Chapter 10 developed ProApriori; an Apriori style algorithm which is based on candidate generation and checking of PFIMs. Chapter 12 improved on this by developing a probabilistic pattern growth approach inspired by the FP-Growth method. Here, a compact representation of the data set as an interlinked tree storing both certain and uncertain occurrences enables faster run times than ProApriori. This chapter uses the GIM framework and algorithm by casting the PFIM problem in terms of vectors and functions of vectors. This mapping is both intuitive and allows the application of the GIM algorithm. The resulting approach, called GIM-PFIM, is shown to be significantly faster and use much less memory than both ProApriori and ProFP-Growth. The improvement in space usage and run time is about an order of magnitude better than ProFP-Growth.

13.1.1 Research Problem and Data Model

This chapter solves the Probabilistic Frequent Itemset Mining (PFIM) problem (definition 10) and the Significant Frequent Itemset Mining (SiFIM) efficiently. There are two parts to these problems:

1. Given the existential probabilities of an itemset in all transactions, calculating the support probability distribution and hence the frequentness probability or the significance of the given itemset.
2. Mine all itemsets that satisfy the frequentness or significance constraints by
   (a) Searching through the space of uncertain itemsets,
   (b) Calculating the required probabilities for 1. and
   (c) Using 1. to determine whether an itemset is interesting (a PFI or a SFI).

This chapter focuses on solving the second part of the problem very efficiently. The PFIM problem is solved by plugging in the methods for computing the frequentness probability (either the Poisson binomial recurrence method of chapter 10 or equivalently the generating function method of chapter 12). The SiFIM problem can be solved by plugging in either of the two significance tests proposed in chapter 11.

The uncertain data model applied in this chapter is based on the possible worlds semantic with existential uncertain items as introduced in chapter 10.

13.1.2 Contributions

This chapter makes the following contributions:

- It shows that the PFIM problem can be cast into the vectorised GIM framework, and hence that it can be solved using the GIM algorithm. The resulting method for solving the PFIM problem, called GIM-PFIM, is orders of magnitude faster and requires orders of magnitude less space than the previous state of the art algorithms for solving PFIM. This chapter is also the first work to evaluate and compare all solutions to PFIM on well known and full sized real world data sets.
- As a side effect, this work strengthens the argument for solutions at the abstract level and further validates the flexibility, efficiency and effectiveness of the GIM framework and algorithm.

13.1.3 Organisation

The remainder of this chapter is organised as follows: Section 13.2 briefly puts this chapter in context, section 13.3 shows how the PFIM problem can be solved with GIM, section 13.4 presents in depth experiments and this chapter concludes in section 13.5.

TID	Transaction t_i
1	$\{a : 0.8,\ b : 0.2,\ d : 0.5,\ e : 1.0\}$
2	$\{b : 0.1,\ c : 0.7,\ d : 1.0\}$
3	$\{a : 0.5,\ d : 0.2,\ e : 0.5\}$
4	$\{d : 0.8, e : 0.2\}$
5	$\{c : 1.0,\ d : 0.5,\ e : 0.8\}$
6	$\{a : 1.0,\ b : 0.2,\ c : 0.1\}$

(a) Uncertain transaction database.

Item v	Sparse Vector x_v	Full Vector x_v
a	$[1 : 0.8, 3 : 0.5, 6 : 1.0]$	$[0.8, 0, 0.5, 0, 0, 1.0]$
b	$[1 : 0.2, 2 : 0.1, 6 : 0.2]$	$[0.2, 0.1, 0, 0, 0, 0.2]$
c	$[2 : 0.7, 5 : 1.0, 6 : 0.1]$	$[0, 0.7, 0, 0, 1.0, 0.1]$
d	$[1 : 0.5, 2 : 1.0, 3 : 0.2, 4 : 0.8, 5 : 0.5]$	$[0.5, 1.0, 0.2, 0.8, 0.5, 0]$
e	$[1 : 1.0, 3 : 0.5, 4 : 0.2, 5 : 0.8]$	$[1.0, 0, 0.5, 0.2, 0.8, 0]$

(b) Vectorised uncertain transaction database.

Figure 13.1: Example uncertain transaction database in terms of vectors. The possible items (variables) are $V = \{a, b, c, d, e\}$ and there are 6 uncertain transactions.

13.2 Related Work

Recall that section 10.2 provided an in depth discussion of work related to frequent itemset mining in uncertain and probabilistic databases. This thesis presented PFIM (the problem was introduced and first solved in the publication [18] and the corresponding chapter 10) and the subsequent major advances in solving this problem efficiently. Therefore, the relevant competing methods have already been presented in chapters 10 and 12. GIM is a novel framework and algorithm based on a vectorised view of interaction mining, and itemset mining is one form of interaction mining. GIM is covered in chapter 3 and has its roots in solving many of the other problems presented in this thesis. Relevant literature on the itemset mining problem can be found in section 4.3.

13.3 Solving PFIM with GIM

PFIM can be cast into the vectorised model proposed by GIM resulting in an intuitive way of thinking about the PFIM problem. A probabilistic frequent itemset (PFI) captures an interaction between items in an uncertain database. In the vectorised GIM view, each item is a variable and each itemset (set of variables) $V' \subset I$ can be represented by a vector $x_{V'}$ in the probability space $X = [0, 1]^{|T|}$ spanned by the uncertain transactions T. In particular, $x_{V'}[i]$ is the probability that the itemset V' is

contained in the ith transaction. Note therefore that $x_{V'}$ provides all the information necessary to compute the frequentness probability (or significance) of the itemset V' using the methods in chapters 10, 11 or 12. The vectors x_v for each uncertain item $v \in I$ are easily read from an uncertain transaction database by recording the existence probabilities $P(c \in t_i)$ in $x_v[i]$. Of course, sparse or compressed formats can be used. Figure 13.1 shows two vector representations of the example database of figure 10.2, first in a sparse format where only those dimensions (transactions) containing the item with a non-zero probability is listed, and the full format where each dimension is recorded.

Under the independence assumption (see chapters 10 and 11 for an explanation and justification), it is easy to compute the interaction vector for a probabilistic itemset as follows: $x_{V'}[i] = \Pi_{v \in V'} x_v[i]$. For example, $x_{\{a,e\}} = [1 : 0.8, 3 : 0.25]$ or in full vector form; $[0.8, 0, 0.25, 0, 0, 0]$. Determining the existence probabilities of $V' \cup v$ when a new item $v \in I$ is added to an existing itemset V' is therefore simply a matter of element-wise multiplication of its vector x_v with the existing $x_{V'}$. Note that due to the operation of GIM, such a vector $x_{V'}$ will have been created previously on the current path of the search. Indeed, recall that the GIM algorithm never recomputes any parts of vectors while using the least amount of space possible. When used for PFIM, this means that the probabilities $\Pi_{v \in V'} P(v \in t_i)$ are computed incrementally by reusing prior results. This contrasts the methods used in ProApriori and ProFP-Growth. Further, note that using the sparse representation, only that subspace where both V' and v exist are recorded. Since this subspace (spanned by the transactions in which $V' \cup v$ have a non-zero probability of existing) becomes smaller as the size of the itemset increases (the space is the intersection of the spaces in which V' and v exist), this further increases both the space and run-time efficiency of the algorithm as it progresses. Furthermore, this automatically prunes away any 0's before the frequentness probability is calculated, removing the need to do this explicitly as part of the certainty optimisation (see for example section 10.4.1.1).

Based on the above discussion, PFIM can be solved in GIM as follows:

- The vectors x_v are defined so that $x_v[i] = P(v \in t_i)$. The order on the variables (items) is arbitrary. Recall that a sparse vector method is most efficient, so only $P(v \in t_i)$ greater than 0 need to be stored.
- $a_I(x_{V'}, x_v)$ is computed so that $a_I(x_{V'}, x_v)[i] = x_{V'}[i] \cdot x_v[i]$. Recall that $x_{V'}[i]$ is the probability that $V' \subseteq t_i$ under the independence assumption.
- $m_I(x_{V'})$ computes the frequentness probability of V' (or the significance level if used for SiFIM).

- $M_I(\cdot)$ is trivial.
- $I_I(\cdot) = S_I(\cdot)$ and returns true if and only if $m_I(x_{V'}) \geq \tau$ (or if the p_{value} is below a given level of significance for SiFIM).

With this instantiation, GIM solves the PFIM (or SiFIM) problem. The resulting algorithm is called GIM-PFIM (GIM-SiFIM). The space requirement is that of the database in sparse format (actually less, since it is easy to avoid storing x_v for any v that is not a PFI). The run time is linear in the number of itemsets that need to be examined, making GIM-PFIM optimal (see theorem 3.8).

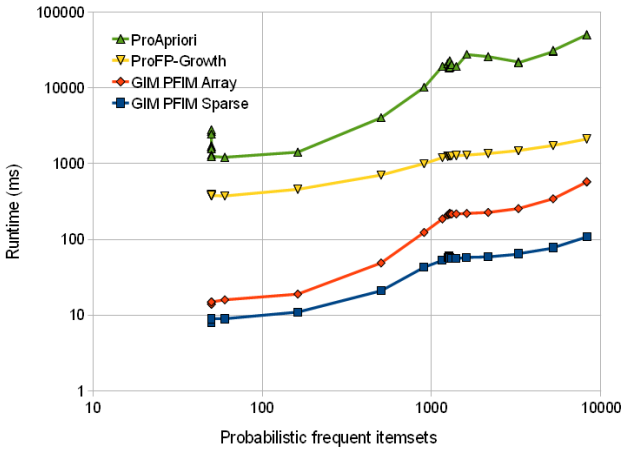
13.4 Experiments

This section experimentally[1] compares GIM applied to the PFIM problem with the previous state of the art methods ProApriori and ProFP-Growth. Both artificial and well known real world data sets were used. All algorithms used the Poisson binomial recurrence computation method with certainty optimisation as outlined in chapter 10. As a side note, all GIM experiments using sparse vectors shown in this section had no problems running on a small netbook with a 1.6GHz Atom processor and default JVM settings ($< 64MB$ RAM). Both ProApriori and ProFP-Growth on the other hand required considerably more computational resources (at least an order of magnitude more). In order to remove the effects of i/o operations, the data sets were retained in memory in the experiments.

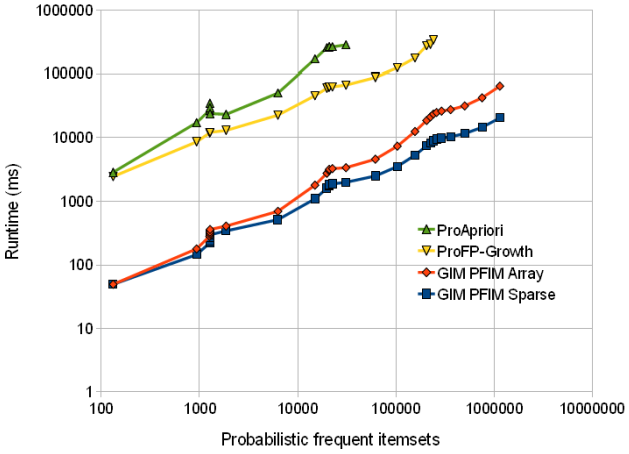
13.4.1 Artificial Data Sets

In order to evaluate the run time on databases with different characteristics, a series of small but representative artificial databases was generated. These consisted of 50 items, 1000 transactions and were generated as follows: First, a certain database was generated by including an item in a transaction with probability p_1 so that on average, each item occurs in p_1 transactions. Then, with probability p_{alter1} the certain occurrences were changed to a uniformly distributed value in $[0, 1]$. p_{alter1} therefore determines the level of uncertainty. The minimum frequentness probability τ was set to 0.9 so that only itemsets were found that are highly likely to be frequent. Note that τ only affects the run time for calculating the frequentness probability. Since all algorithms use exactly the same evaluation, little is gained from varying τ.

[1] Experiments were performed on an Opteron Dual Core * 2, 2.6GHz, 32GB RAM computer running SuSE-Linux 10.2 and Java 1.6. One core was utilised.



(a) $p_1 = 0.25$, $p_{alter} = 0.5$



(b) $p_1 = 0.5$, $p_{alter} = 0.5$. Experiments were aborted once the comulative time hit 30 minutes.

Figure 13.2: Run time results on artificial data sets.

Furthermore, the run time results would be similar for SiFIM (chapter 11) or for the expected support method (except that all algorithms would be a little faster). By varying *minSup*, it is possible to generate a graph showing the run time behaviour of the algorithms in terms of the number of probabilistic frequent itemsets mined. Figure 13.2 shows the performance of ProApriori, ProFP-Growth and GIM-PFIM (showing both sparse and non-sparse vector implementations). ProFP-Growth is faster than ProApriori, as expected from previous results. GIM-PFIM however is at least an order of magnitude faster than both. Furthermore, it can be seen that the sparse vector implementation further improves the run time efficiency, and this effect increases as the number of itemsets mined increases. Recall that sparse methods corresponds to mining projected subspaces. As the size of the probabilistic frequent

itemsets increase, they define smaller and smaller subspaces that need to be mined. Hence the vectors become smaller and operations on these become faster.

The wave like effect that can be observed over the orders of magnitude is likely due to the way the data sets were generated[2].

13.4.2 Well Known and Real World Databases

The algorithms were also evaluated on two large, publicly available data sets: The well known FIM database (T10I4D100K) consisting of 870 items and 100,000 transactions; and the real world retail data set with 16,470 items and 88,162 transactions. Both are available from the FIM data set repository [39]. Being certain data sets, these were altered as above to generate various uncertain databases. p_{alter1} was varied to values in $\{0, 0.25, 0.5, 0.75, 1\}$, where $p_{alter1} = 0$ corresponds to the data set remaining certain, and $p_{alter1} = 1$ corresponding to a completely uncertain database where no item exists for certain in any transaction. In the graphs, p_{alter1} is denoted by $P(Alter1)$. GIM was used with sparse real vectors only.

T10I4D100K

Figures 13.3 and 13.4 show the results on the T10I4D100K data set. Again, $minSup$ was varied from 1000 to 2 to obtain the graph. The total time allowed for each series of experiments (line in the graph) was limited however; 30 minutes for GIM, and 2 hours for ProFP-Growth and ProApriori. In the completely uncertain data set and for the lowest $minSup$ setting ($minSup = 2$), ProFP-Growth achieves the same run time as GIM. However, this setting corresponds to a support of only 2 out of the 100,000 transactions, or 0.002%. Furthermore, it generates far too many probabilistic frequent itemsets to be useful. When there is less uncertainty, this crossover point increases to $minSup = 17$, or 0.017%. Such settings are pointless in practice, where higher support is desired. It can clearly be seen that regardless of the level of uncertainty in the data set, GIM outperforms ProFP-Growth for practical levels of $minSup$, usually by one order of magnitude. ProApriori is over an order of magnitude slower than ProFP-Growth, and at least two orders of magnitude slower than GIM.

[2]Since the probabilities were generated from the same distribution, all itemsets of size k can be expected to have similar probabilities of being frequent but the larger the itemsets become, the smaller their existence probabilities but the more of them there are. Further, the random number generator is not a particularly robust. These effects lead to ranges for $minSup$ where many itemsets must be examined while few are interesting, and other settings (when $minSup$ is increased above a certain threshold) where suddenly a higher percentage of the itemsets examined end up being probabilistically frequent.

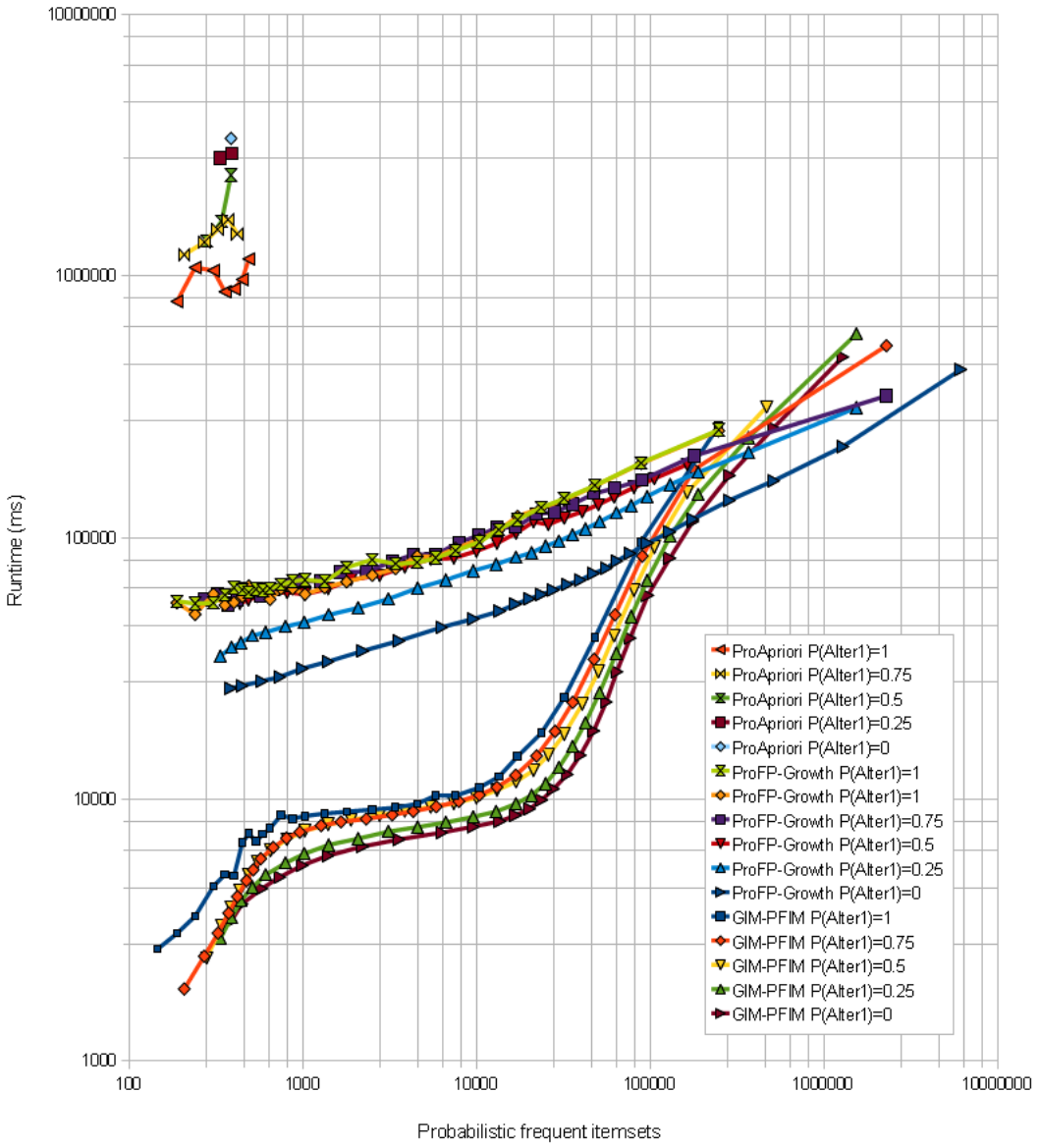
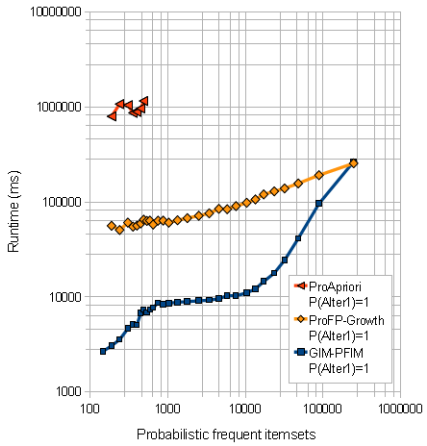
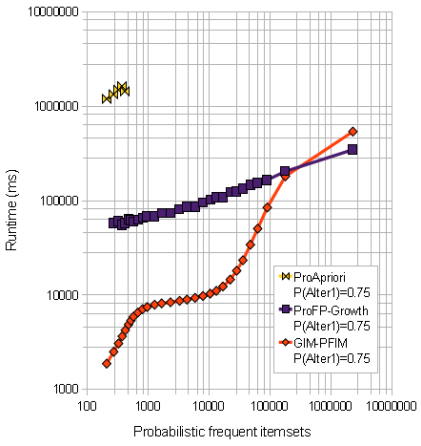


Figure 13.3: Run time results on the uncertain T10I4D100K data set. The results are split up by p_{alter1} value in figure 13.4.

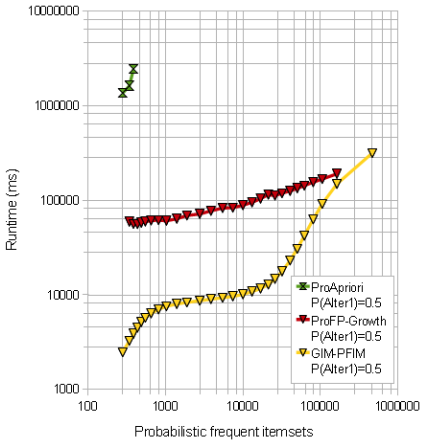
There is also a large difference in memory required between GIM and ProFP-Growth. All the GIM experiments ran on the default JVM settings and required at most 48MB of RAM. ProFP-Growth on the other hand, required up to about 7.4GB of RAM – over one order of magnitude more. ProApriori generally used a few GB of RAM. Incidentally, all GIM experiments happily run on a small netbook with the same run time characteristics, albeit at a constant factor slower due to the slower CPU.



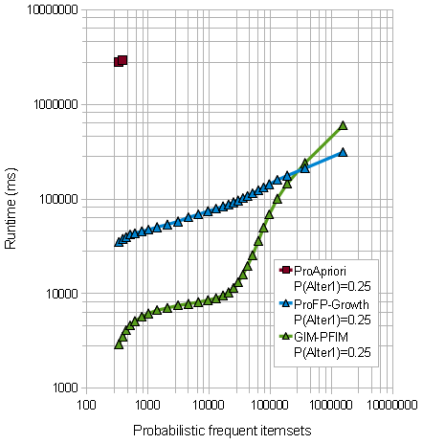
(a) $p_{alter} = 1$. Crossover point at $minSup = 0.002\%$



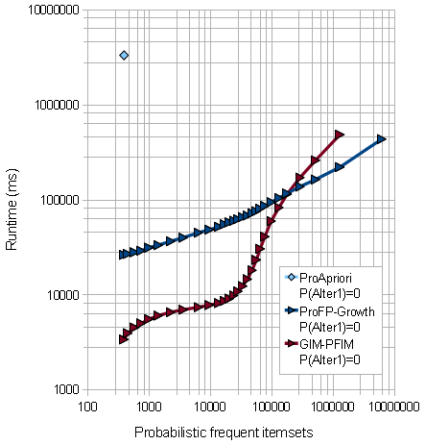
(b) $p_{alter} = 0.75$.



(c) $p_{alter} = 0.5$.



(d) $p_{alter} = 0.25$.



(e) $p_{alter} = 0$. Crossover point at $minSup = 0.017\%$

Figure 13.4: Run time results on the uncertain T10I4D100K data set, showing each setting for p_{alter1}.

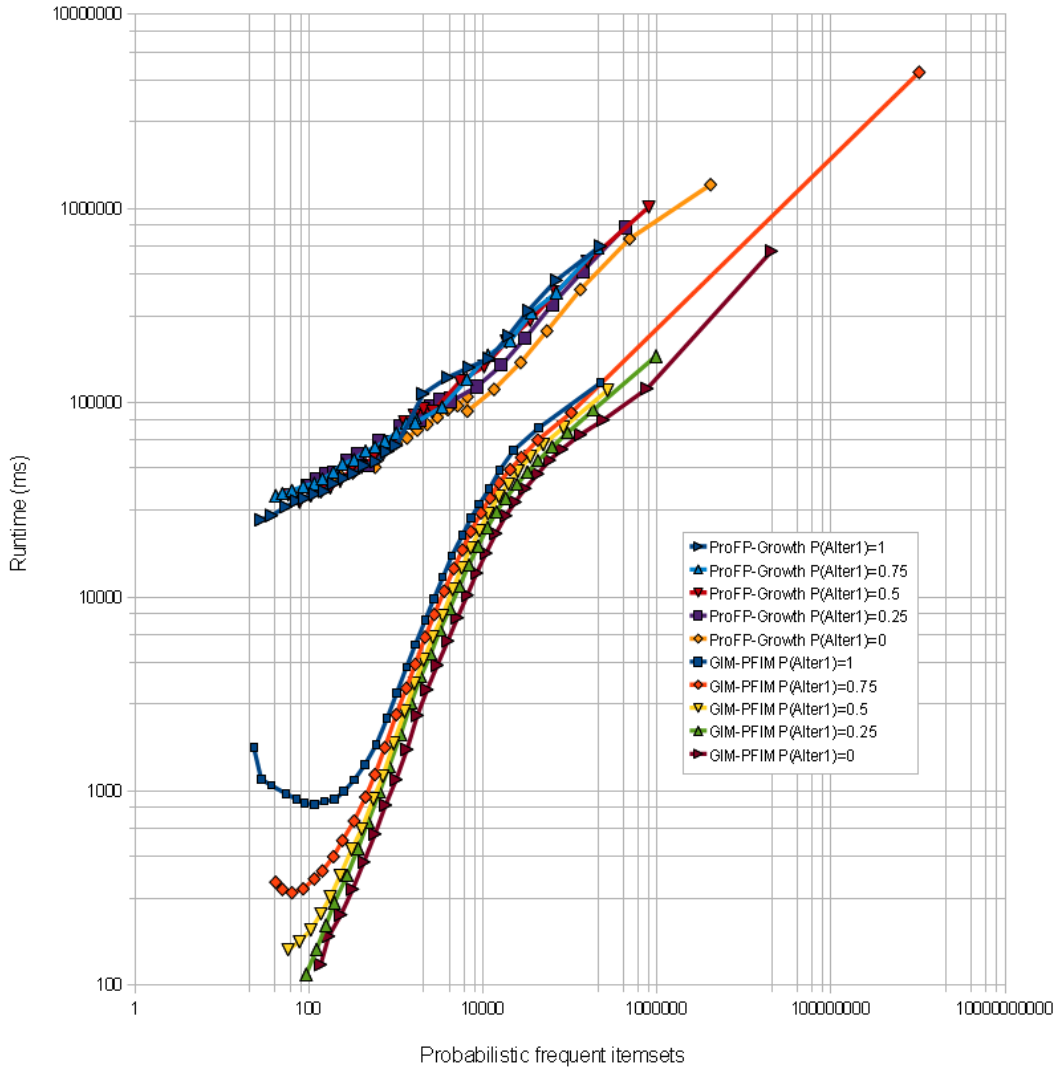


Figure 13.5: Run time results on the full uncertain retail data set.

Retail

Figure 13.5 show the run time results on the retail data set. While T10I4D100K had few items in comparison to the number of transactions (870/100000 = 0.87%), the retail data set has over an order of magnitude more items (16,470/88126 = 18.7%) while still having a large number of transactions (88% of those in T10I4D100K). It therefore provides a more challenging test in addition to an evaluation on a real world data set. Again, *minSup* was varied as described above, but ProFP-Growth had to be run for an extra 2 hours per line in order to get the results displayed. ProApriori failed to run on the retail data set; most likely due to the high number of items causing too many candidates to be generated; even with the JVM set to allow up

to 20GB or RAM. The results clearly show that GIM-PFIM is superior to ProFP-Growth for all *minSup* settings and all levels of uncertainty. The improvement ranges up to over 2 orders of magnitude.

13.5 Conclusion

Probabilistic frequent itemset mining (PFIM) is a challenging problem, requiring both efficient computation of the support probability distribution, and algorithms able to mine all probabilistic itemsets efficiently. This chapter presented the fastest and most efficient algorithm to date for PFIM. It beats the previous state of the art algorithms by at least an order of magnitude. In addition, the results in this chapter lend weight to the wide ranging applicability, effectiveness and efficiency of the GIM framework and algorithm.

Part V

Conclusions

Chapter 14

Conclusions and Future Work

This thesis was organised into three main research themes: Part II considered various interaction mining problems and proposed novel solutions at the abstract level via generalised frameworks and an efficient vectorised computation model. Part III considered the integration of rigorous statistical approaches in novel data mining methods, and part IV proposed and solved the problem of mining probabilistic frequent itemsets in uncertain databases.

Uncertain or probabilistic databases pose significant challenges for the KDD process. They require the development of specialist algorithms that take into account the probability distributions of the data in order to deliver useful results to the user. This was demonstrated in the context of frequent itemset mining, where existing work treated itemsets as being interesting if their expected support was high. This is known as the expected FIM (EFIM) problem. While the EFIM approach lead to the relatively easy extension of FIM algorithms, it has the fundamental flaw that it provides no confidence in the result. Indeed, it was shown in this thesis that it leads to scenarios where itemsets are labeled frequent even if they are actually more likely to be infrequent. It was also demonstrated that the expected support approach labeled many patterns interesting in a random database, even though these patterns were statistically insignificant. Clearly, this is undesirable.

In response to these problems, part IV of this thesis proposed and solved the Probabilistic Frequent Itemset Mining (PFIM) problem, where itemsets are considered interesting if the *probability* that they are frequent is high. PFIM delivers high quality patterns and does not suffer the downsides of EFIM since it uses the probability distribution of an itemset's support. This methodology made the problem much more challenging however. In particular, two problems needed to be addressed:

First, an efficient method was required to calculate an itemset's support probability distribution (SPDF) and frequentness probability. This thesis used the possible worlds model and a proposed probabilistic framework to solve this problem in various ways: Novel methods based on the Poisson binomial recurrence (chapter 10) and generating functions (chapter 12) were developed. Despite calculating the exact SPDF and frequentness probability, these avoided the exponential run time of naive solutions and had run times close to the EFIM method. Approximate results using a Normal approximation are also investigated (chapter 11). Secondly, novel algorithms needed to be developed in order to efficiently calculate and feed itemsets' existence probabilities to the frequentness probability computation method, and in turn search through the space of itemsets. Since more probability information is required in comparison to EFIM, specialist algorithms had to be developed. This thesis first developed ProApriori, which is based on the candidate generation and testing framework (chapter 10). Then, ProFP-Growth was proposed in chapter 12. This was the first probabilistic FP-Growth type algorithm and used a proposed probabilistic frequent pattern tree (Pro-FPTree) to avoid candidate generation, while being able to compress the uncertain transaction database in a loss-less manner. Finally, the PFIM problem was mapped to the GIM framework, casting PFIM as a vectorised interaction mining problem in chapter 13. The resulting GIM-PFIM algorithm is the current fastest known algorithm for solving the PFIM problem. In comparison to ProApriori and ProFP-Growth, it achieved orders of magnitude improvements in space and time usage. Furthermore, it lead to an intuitive subspace and probability-vector based interpretation of PFIM. Incremental methods were also proposed to answer queries such as finding the top-k probabilistic frequent itemsets.

This thesis identified a fundamental problem with the prior state of the art approach to mining itemsets in uncertain databases, proposed an alternative approach that overcame these problems and examined it in depth. This demonstrates the need and advantages of developing specialist algorithms that take account the probability distribution of the target measure in uncertain or probabilistic databases. It also showed that doing so can not only lead to higher quality output for the user, but very efficient algorithms. This thesis contributed a range of methods that efficiently find high quality probabilistic frequent patterns in uncertain or probabilistic databases, potentially rendering the previous expectation based method obsolete.

Another hypothesis considered in this thesis was that statistical techniques embedded within data mining and machine learning methods lead to better descriptive and predictive outcomes. Therefore, significance tests and Pearson's correlation were used to develop various novel data mining approaches. The use of significance tests

was based on the observation that data mining is a hypothesis generating endeavour, and that DM algorithms make decisions in their search for interesting patterns. Since the database is a sample, the patterns found should describe hypotheses about the underlying process that generated the data. Furthermore, a DM algorithm should ideally deliver patterns that are statistically significant, so that they are unlikely to have occurred by chance, noise or sampling effects. Finally, the decisions made by an algorithm during its search should ideally also be significant, so that the search itself is not sensitive to 'chance'. These issues are often ignored. It is desirable to provide some minimal level of confidence that the patterns found are in fact significant, and that the algorithm does not make decisions likely to have occurred by chance. Post processing is not an effective solution to these problem for two reasons: First, it cannot address the issue of significant algorithmic decisions. Secondly, it means that what the user is ultimately interested in (the knowledge provided at the output of post-processing) is not what the data mining algorithm is actually searching for. At best, this is very inefficient. At worst, the algorithm never finds those patterns that the post-processing task would rate most highly.

One method used in this thesis to mine significant patterns is to use significance tests within the search and interestingness measures themselves. This means that both the decisions made by the search, as well as the patterns found, have high confidence. This approach was used in chapter 8, which addressed the problem of rule based classification of standard and in particular, highly imbalanced (skewed) data sets. Mining data sets with an imbalanced class distribution is challenging and is required in applications such as medical diagnosis and fraud detection. In the proposed SPARCCC method, rules are interesting if they have a positive class correlation ratio, are statistically significant based on Fisher's exact test and are positively associated. The search also progresses based on significance tests and therefore mines significant rules directly. In contrast, many other associative classification methods were based on the support framework and subsequent filtering. This was found to lead to rules with a bias against the minority class, rules that were statistically insignificant or could be correlated more highly with an alternative class to the one they predict. By relying on the popular support-confidence framework and filtering the results in post processing, these methods were also very inefficient; requiring that many rules be mined but discarding up to 99% of them in order to achieve acceptable classification performance. SPARCCC on the other hand achieved the same accuracy on balanced data sets and much higher classification performance on imbalanced data sets, discovered orders of magnitude fewer – but high quality – rules and discarded none of them.

A second method to deliver only significant results is to mine patterns that are interesting with a high probability; that is, to generate a significance test around an existing interestingness measure. This approach is taken in chapter 11, where itemsets are mined if they are significantly frequent. Again, a non-parametric method was used and the results had a higher quality than the alternative expectation approach.

Finally, Pearson's product moment correlation coefficient was used in a number of novel methods in this thesis. Chapter 9 considered the problem of mining complex maximal cliques of correlated variables (attributes) for the purpose of feature selection, meaningful dimensionality reduction, and as an interaction mining technique in its own right. An efficient algorithm was developed based on a proven structural constraint on complex correlation graphs. Correlation was also used successfully for mining correlated multiplication rules for interaction mining and feature generation; and conjunctive correlation rules for classification.

Together then, these results support the hypothesis that better predictive and descriptive patterns are mined by the incorporation of statistical techniques embedded directly within novel data mining methods.

This thesis developed a range of data mining methods that can be covered by the term *interaction mining*. While solving these problems, it was discovered that many aspects were similar when regarded from a suitably abstracted view: In general, a data set can be considered as a set of variables about which one has samples. Interaction mining is the process of mining structures on these variables that describe interaction patterns. Usually, these structures can be represented as sets or graphs; where each variable interacts, to some degree, with other variables in the structure. Such interactions can also be complex, representing both positive and negative relationships, and can include negative patterns. Furthermore, the presence of particular interactions can influence another interaction or variable in interesting ways. These latter kinds of interactions can be expressed as rules. Recall that interactions are of interest in many domains, ranging from social network analysis, marketing, the sciences, to statistics and finance. Furthermore, many data mining tasks can be considered as mining interactions, such as clustering, frequent itemset mining, rule based classification, graph mining, etc.

Therefore, the research problem was to develop abstract frameworks, a computational model and algorithms capable of modeling, capturing and solving a wide range of such interaction mining problems at the abstract level, and to do so very efficiently. This was a challenging task since such problems have very different semantics governing the interactions, their structures and their interpretation: The pattern definitions

and semantics are different; what makes an interaction pattern interesting is different; how the search should progress is different and the data is also very different. Finally, solving interaction mining problems usually requires the simultaneous and interdependent development of new pattern semantics and specialist algorithms for mining the respective pattern. One can therefore conclude that it is not easy to develop models abstract enough to capture this variation in interaction mining problems, while at the same time enabling the development of equally abstract algorithms that also solves them efficiently – ideally, more efficiently than specialist algorithms. But this is what part II of this thesis achieved:

Chapter 3 introduced and solved the GIM problem. GIM uses an efficient and intuitive computational model based purely on vectors and vector valued functions. The semantics of the interactions, their interestingness measures and the type of data considered are all flexible components. Intuitively, each interaction is represented by a vector in a space typically spanned by the samples in the database. The search progresses by performing functions on these vectors. The GIM algorithm runs in linear time in the number of interesting interactions and uses little space. Chapter 3 showed how GIM can be applied to a wide range of problems, including graph mining, counting based methods, itemset mining, clique mining, clustering, complex pattern mining, negative pattern mining, solving an optimisation problem, etc. Later, it was shown that it can solve many of the problems considered in other parts of this thesis. For example, it turns out to be the most efficient solution to the PFIM problem considered in part IV. It can also solve the problems considered in chapter 9 and 5. Other interaction mining problems considered in this thesis are covered in chapters 4 and 5. Chapter 4 presented a vectorised framework and novel algorithm called GLIMIT for solving abstract itemset mining problems from a geometric perspective in a transposed database. It is shown to outperform FP-Growth and Apriori on the frequent itemset mining task. An efficient method for generating association rules was also presented. Chapter 5 considered the problem of mining complex co-location patterns between different types of objects in a real world spatial database. When applied to a large astronomy database, this mines relationships – including negative relationships and the effect of multiple occurrences – between different *types* of galaxies. Part of this problem was solved with GLIMIT but can be solved directly with GIM.

Chapter 6 introduced and solved the Generalised Rule Mining (GRM) problem. Rules are an important interaction pattern but existing approaches were limited to conjunctions of binary literals, fixed measures and counting based algorithms. Rules can be much more diverse, useful and interesting! The chapter redefined rule mining

in terms of a similar vectorised computational model to that used in GIM. This abstraction was motivated through the introduction of three diverse and novel methods addressing problems including correlation based classification, finding interactions for improving regression models and finding probabilistic association rules in uncertain databases. Two of these methods were introduced in chapter 6 (Probabilistic Association Rule Mining (PARM) in uncertain databases and Conjunctive Correlation Rules (CCRules) for classification), while one was introduced in chapter 7. Furthermore, the SPARCCC method can also be solved with GRM, as was outlined in chapter 8. Since interactions between variables in a database are often unknown to the detriment of further analysis, classification or mining tasks, chapter 7 proposes Correlated Multiplication Rules (CMRules). These capture interactions predictive of a dependent variable and are the first rules with multiplicative semantics. Furthermore, a feature selection and dimensionality reduction method was described whereby CMRules are used to generate composite features. One advantage of this is that it enables linear models to learn non-linear decision boundaries with respect to the original variables.

In summary then, in addition to proposing and solving the PFIM problem and developing useful methods based on statistical approaches in data mining, this thesis successfully abstracted and solved the problem of mining interactions between variables. The interaction mining problem was solved through the development of abstract frameworks and algorithms operating on a vectorised computational model. By doing this, one can separate the semantics of an interaction mining problem from the algorithm used to mine it, allowing both to vary independently of each other. This makes it easier to develop new methods by allowing the data miner to focus only on their problem's semantics and then plug them into a framework. Furthermore, the frameworks make it easy to push good interestingness measures (such as significance tests and correlation) directly into the mining process. This leads to higher quality results, more efficient solutions and less reliance on measures that are traditionally easier to implement but are not necessarily correlated with predictive or descriptive performance (for example, support). Examples where these aspects were demonstrated in this thesis include chapters 3, 5, 6, 7, 8, 9 and 13. Results in this thesis also suggest that forcing good quality interestingness measures (that correlate with the user's utility) to be anti-monotonic to allow for effective pruning when they do not naturally have pruning friendly properties (for example, using the *improvement* methods described in chapter 3 and 6), gives much better results than using interestingness measures that are not directly related to the users utility, but allow good pruning.

By removing the burden of designing an efficient algorithm, it is also easier for end users to design custom data mining algorithms. By allowing the algorithms to vary independently of the problem, new ones can be developed that can be immediately be applied to solve many problems. Since it was shown that all problems considered in this thesis can (at least retrospectively) be mapped to and solved by GIM or GRM, any new GIM or GRM algorithm can immediately speed up all of these problems without specialisation or modification. This property is particularly advantageous when DM is embedded into practical applications. The GIM and GRM algorithms are already efficient however, achieving the asymptotically optimal linear run time in the number of interactions that must be examined and using little space. When applied to specific problems, they turned out to be most efficient. For example, the PFIM problem was solved not only most efficiently, but also most intuitively using the GIM framework.

The vectorised computational model introduced in this thesis also encourages an interesting geometric way of thinking about pattern mining problems in terms of vector operations and subspaces – especially when an interestingness measure has a geometric interpretation. Such a geometric interpretation leads to new insights and can inspire new methods. For example, mining rules based on reducing the angle between a vector representing the antecedent and the vector representing the consequent. This idea was used successfully in chapters 6 and 7. Developing methods that are now possible are also fruitful avenues for future work. For example, prior to the development of GRM, multiplication rules were never considered and could not be mined with existing methods. However, their use in chapter 7 turned out to be useful for feature generation and interaction mining. Evaluating this application further is a candidate for future work. GIM also provided a novel vector and subspace-search interpretation of the search for interesting patterns. For example, this was discussed in the context of probabilistic databases. There is plenty of scope for the evaluation of other existing or novel methods using the GIM and GRM frameworks. For example, recall that it was shown in chapter 3 that GIM may be used to solve a wide range of problems, from itemset mining to complex pattern mining to clustering to graph mining to optimisation. Later in the thesis, a number of these problems were considered in detail, together with experimental evaluations and comparison to the state of the art where applicable. Evaluating the others in depth, or developing new methods inspired by the vectorised framework are also promising directions for future work.

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