Exploiting Prior Knowledge and Latent Variable Representations for the Statistical Modeling and Probabilistic Querying of Large Knowledge Graphs

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Hiermit erkläre ich an Eidesstatt, dass die Dissertation von mir selbstständig, ohne unerlaubte Beihilfe angefertigt ist.

Denis Krompaß

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Ort, Datum Unterschrift Doktorand

Formular 3.2

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Abstract

Large knowledge graphs increasingly add great value to various applications that require machines to recognize and understand queries and their semantics, as in search or question answering systems. These applications include Google search, Bing search, IBM's Watson, but also smart mobile assistants as Apple's Siri, Google Now or Microsoft's Cortana. Popular knowledge graphs like DBpedia, YAGO or Freebase store a broad range of facts about the world, to a large extent derived from Wikipedia, currently the biggest web encyclopedia. In addition to these freely accessible open knowledge graphs, commercial ones have also evolved including the well-known Google Knowledge Graph or Microsoft's Satori. Since incompleteness and veracity of knowledge graphs are known problems, the statistical modeling of knowledge graphs has increasingly gained attention in recent years. Some of the leading approaches are based on latent variable models which show both excellent predictive performance and scalability. Latent variable models learn embedding representations of domain entities and relations (representation learning). From these embeddings, priors for every possible fact in the knowledge graph are generated which can be exploited for data cleansing, completion or as prior knowledge to support triple extraction from unstructured textual data as successfully demonstrated by Google's Knowledge-Vault project. However, large knowledge graphs impose constraints on the complexity of the latent embeddings learned by these models. For graphs with millions of entities and thousands of relation-types, latent variable models are required to exploit low dimensional embeddings for entities and relation-types to be tractable when applied to these graphs.

The work described in this thesis extends the application of latent variable models for large knowledge graphs in three important dimensions.

First, it is shown how the integration of ontological constraints on the domain and range of relation-types enables latent variable models to exploit latent embeddings of reduced

complexity for modeling large knowledge graphs. The integration of this prior knowledge into the models leads to a substantial increase both in predictive performance and scalability with improvements of up to 77% in link-prediction tasks. Since manually designed domain and range constraints can be absent or fuzzy, we also propose and study an alternative approach based on a local closed-world assumption, which derives domain and range constraints from observed data without the need of prior knowledge extracted from the curated schema of the knowledge graph. We show that such an approach also leads to similar significant improvements in modeling quality. Further, we demonstrate that these two types of domain and range constraints are of general value to latent variable models by integrating and evaluating them on the current state of the art of latent variable models represented by RESCAL, Translational Embedding, and the neural network approach used by the recently proposed Google Knowledge Vault system.

In the second part of the thesis it is shown that the just mentioned three approaches all perform well, but do not share many commonalities in the way they model knowledge graphs. These differences can be exploited in ensemble solutions which improve the predictive performance even further.

The third part of the thesis concerns the efficient querying of the statistically modeled knowledge graphs. This thesis interprets statistically modeled knowledge graphs as probabilistic databases, where the latent variable models define a probability distribution for triples. From this perspective, link-prediction is equivalent to querying ground triples which is a standard functionality of the latent variable models. For more complex querying that involves e.g. joins and projections, the theory on probabilistic databases provides evaluation rules. In this thesis it is shown how the intrinsic features of latent variable models can be combined with the theory of probabilistic databases to realize efficient probabilistic querying of the modeled graphs.

Zusammenfassung

Wissensgraphen spielen in vielen heutigen Anwendungen wie Websuche oder automatischen Frage-Antwort-Systemen eine bedeutende Rolle. Dabei werden Maschinen von Wissensgraphen darin unterstützt, die Kernaspekte der Semantik von Benutzeranfragen zu erkennen und zu verstehen. Prominente Beispiele, in denen die Integration von Wissensgraphen einen beachtlichen Mehrwert geliefert hat, sind Googles und Microsofts Websuche sowie IBMs Watson. Im mobilen Bereich sind vor allem auch diverse Assistenzsysteme wie Google Now, Apple Siri und Microsoft Cortana nennenswert. Die wahrscheinlich bekanntesten Wissensgraphen sind der kommerziell genutzte Google Knowledge Graph und Microsofts Satori, die vor allem die Websuche unterstützen. Freebase, DBpedia und YAGO gehören zu den bekanntesten Beispielen für Wissensgraphen, die einen freien Zugriff auf ihre Daten erlauben. Diese Graphen haben gemeinsam, dass sie eine breite Sammlung von Fakten speichern, die zu einem großen Teil von Wikipedia stammen, der momentan größten verfügbaren Web-Enzyklopädie. Trotz des großen Mehrwerts, den diese Graphen bereits heute erbringen, gibt es einige Aspekte, die zu Einschränkungen und Problemen bei der Anwendung führen. Zu diesen Aspekten gehören vor allem Unsicherheit und Unvollständigkeit der gespeicherten Fakten. Statistisch motivierte Verfahren zur Modellierung dieser Graphen stellen einen Ansatz dar um diese Probleme zu adressieren. Dabei haben sich insbesondere *Latent Variable Models*, die zum Bereich des Repräsentations-Lernens gehören, als sehr erfolgversprechend erwiesen. Diese Modelle lernen latente Repräsentationen für Entitäten und Relationen, aus denen Schlussfolgerungen über die Richtigkeit für jede mögliche Relation zwischen Entitäten abgeleitet werden können. Diese Schlussfolgerungen können dazu benutzt werden bestehende Wissensgraphen aufzubereiten, zu vervollständigen oder sogar um die automatische Konstruktion von neuen Wissensgraphen aus unstrukturierten Freitexten zu unterstützen, wie es im kürzlich veröffentlichten Google

Knowledge Vault Projekt demonstriert wurde.

Die Modellierung von sehr großen Wissensgraphen stellt eine zusätzliche Herausforderung für diese Modelle dar, da die Größe des modellierten Graphen direkten Einfluss auf die Komplexität und damit auf die Trainingszeit der Modelle hat. Wissensgraphen mit Millionen von Entitäten und Tausenden von unterschiedlichen Arten von Relationen erfordern es, dass die Latent Variable Models mit niedrigdimensionalen latenten Repräsentationen für Entitäten und die verschiedenen Relationen auskommen müssen.

Diese Doktorarbeit erweitert die Anwendung von Latent Variable Models auf große Wissensgraphen in Bezug auf drei wichtige Aspekte.

Erstens, die Integration von Vorwissen über die Semantik von Relationen in Latent Variable Models führt dazu, dass die Graphen mit niedrigdimensionalen latenten Repräsentationen besser modelliert werden können. Dieses Vorwissen steht in Schema-basierten Wissensgraphen oft zur Verfügung. Dabei konnten durch die Berücksichtigung dieses Vorwissens erhebliche Verbesserungen von bis zu 77% bei der Vorhersage von neuen Verbindungen im Graphen erzielt werden. Zusätzlich wird ein alternativer Ansatz vorgestellt, eine Annahme der lokalen Weltabgeschlossenheit, der angewendet werden kann wenn Vorwissen über die Semantik von Relationen nicht verfügbar oder ungenau ist. Durch diese Annahme kann die Semantik von Relationen auf Basis der vorhandenen Fakten im Graph abgeschätzt werden und ist damit unabhängig von einem vorgegebenen Schema. Es wird gezeigt, dass dieser Ansatz ebenfalls zu einer erheblichen Verbesserung in der Vorhersage-Qualität führt. Ferner wird argumentiert, dass beide Arten des Vorwissens über die Semantik von Relationen, zum Einen extrahiert aus dem Schema des Wissensgraphen, zum Anderen abgeleitet von der Annahme der lokalen Weltabgeschlossenheit, generell essentiell für Latent Variable Models zur Modellierung von großen Wissensgraphen ist. Zu diesem Zweck werden beide Arten von Vorwissen in drei Modelle, die den Stand der Technik repräsentieren integriert und untersucht: die Latent Variable Models RESCAL, TransE und das neuronale Netz, welches im Google Knowledge Vault Projekt verwendet wurde.

Die oben genannten drei Modelle haben durch Integration von Vorwissen eine gute Vorhersage Qualität, modellieren jedoch den Wissensgraphen auf sehr unterschiedliche Art und Weise. Für den zweiten Aspekt wird gezeigt, dass diese Unterschiede zwischen den Modellen in Ensemble-Methoden ausgenutzt werden können um die Vorhersage Qualität weiter zu verbessern.

Der dritte und letzte Aspekt, der in dieser Arbeit beschrieben wird, behandelt die effiziente Abfrage von statistisch modellierten Wissensgraphen. Zu diesem Zweck wird der

statistisch modellierte Wissensgraph als probabilistische Datenbank interpretiert, wobei das Latent Variable Model die Wahrscheinlichkeitsverteilung der repräsentierten Fakten definiert. Ausgehend von dieser Interpretation kann die übliche Vorhersage von neuen Verbindungen im Graphen mit den Latent Variable Models als eine Abfrage dieser Datenbank nach einzelnen einfachen Fakten aufgefasst werden. Für komplexere Abfragen, die zum Beispiel Joins oder Projektionen beinhalten können, stellt die Theorie der probabilistischen Datenbank Auswertungsregeln bereit. Es wird gezeigt, wie wesentliche Eigenschaften der Latent Variable Models mit der Theorie der probabilistischen Datenbanken kombiniert werden können um das effiziente Abfragen der statistisch modellierten Wissensgraphen zu ermöglichen.

Chapter 1

Introduction

The rapidly growing Web of Data, e.g., as presented by the Semantic Web's linked open data cloud (LOD) [6], is providing an increasing amount of data in form of large triple databases, also known as triple stores. The main vision of the Semantic Web is to create a structured Web of knowledge from the content of the World Wide Web. The organization of this structured knowledge can be distinguished in two different ways, by schema-free or schema-based graph-based knowledge bases. In schema-free knowledge graphs open information extraction techniques (OpenIE) [29, 30] identify entities and relations from text documents and represent them by their surface names, that is the corresponding string from the textual data. This approach has the advantage that no predefined vocabulary is needed, but the entities and relation-types often lack proper disambiguation, e.g. the system might not explicitly represent the knowledge that "Angela Kasner" and "Angela Merkel" refer to the same real-world entity. In schema-based knowledge graphs on the other hand, one aims to represent entities and relation-types by unique global identifiers. This representation also stores the surface names of entities as literal entities, but in the best case all surface names that refer to the same real-world entity are properly disambiguated through linking them to the same unique global identifier. In Freebase [8] for example, "Angela Kasner" and "Angela Merkel" both refer to the Freebase identifier `/m/0jl0g`. Additionally, all entities and relation-types are predefined by a fixed vocabulary which is often semantically enriched in not necessarily hierarchical ontologies. Through the semantics, entities become real-world things like persons or cities that have various types of relationships and are often enriched with a large amount of additional information that further describe them and their meaning. The Freebase entity with identifier `/m/0jl0g` (Angela Merkel) for example belongs to the class person and is the current chancellor of Germany, where chancellor is

a governmental position. This kind of semantically rich description of real-world entities adds great value to various applications such as web-search, question answering and relation extraction. In these applications, entities and relation-types can be recognized by machines and additional background knowledge can be acquired that better represents the intention of the user. The Google Knowledge Graph is certainly the most famous example, where such approach significantly improved the quality and user experience in web-search.

Today, hundreds of different knowledge graphs have emerged, which represent in part domain specific (e.g. the Gene Ontology [2]), but also general purpose (e.g. Freebase) knowledge. Besides academic efforts to construct large and extensive knowledge graphs like Freebase, DBpedia [66], Nell [16] or YAGO [46], also commercially ones have evolved including Google's and Yahoo!'s Knowledge-Graph or Microsoft's Satori. Based on automated knowledge extraction methods and partially also thanks to a large number of volunteers that are contributing facts and perform quality control, some of the knowledge graphs contain billions of facts about millions of entities, which are related by thousands of different relation-types. Due to the effort of the linked open data initiative, entities have been additionally interlinked between different knowledge graphs, allowing an easier integration of knowledge from different sources of the linked open data cloud. Especially the possibility to combine different sources of information allows machines to consider more diverse information and to better understand the notion of a given task, leading to improved and new applications and services. Today, knowledge graphs power a various set of commercial applications including well known search engines such as Google, Bing, Yahoo or Facebooks's Graph search, but also smart question answering systems such as the IBM Watson [34] system, Apple's Siri or Google Now.

Many knowledge graphs obtain semi-structured knowledge from Wikipedia[1], the currently largest web encyclopedia, which solely relies on a large community of human voluntary contributors that add and edit knowledge to the repository. In addition, other sources of information with varying quality and completeness are integrated, sometimes sacrificing exhaustive quality control management to completeness.

Even though the available knowledge graphs have reached an impressive size, they still suffer from incompleteness and contain errors. Additionally, the amount of contributions of human volunteers is limited, decreasing with the size of the knowledge graph [101]. In Freebase and DBpedia a vast amount of persons (71% in Freebase and 66% in DBpedia) are missing a place of birth [25, 54]. In DBpedia 58% of the scientist do not have a fact that

[1] https://www.wikipedia.org/

describe what they are known for and 40% of the countries miss a capital. Also, information can be outdated and facts can be false or contradicting. Due to the current size of prominent knowledge graphs, exhaustive human reviewing of the represented knowledge has become infeasible and resolving errors and contradictions often remains limited to popular entries which are frequently queried. Contradicting to this observation is the common practice that potentially erroneous new facts, which have not been edited or deleted in a period of time, are assumed to be correct and remain in these database for a very long time until detected [102]. In other words, it is expected that the error rate in unpopular entries is much higher than in the more popular ones, and these errors are persistent.

Due to these problems, methods for the automatic construction of knowledge graphs have emerged as a research field of their own. Especially approaches that evaluate the quality of existing facts, detect errors, reason about new facts, and extract high quality knowledge from unstructured text documents, are desired. Most of the knowledge contained in e.g. Wikipedia is hidden in the free-text description of the articles and only a small part of general information is covered by the Infoboxes which are primarily mined by larger knowledge graphs like DBpedia, Freebase or YAGO. The NELL (Never-Ending Language Learning) project [16] is one example, where a knowledge repository is continuously extended through a web reading algorithm. In the Google Knowledge Vault system [25], the relations extracted from a large corpus of unstructured text are combined with prior knowledge mined from existing knowledge graphs (Freebase) to automatically extract high confidence facts. This prior knowledge is in part derived by statistical models of existing knowledge graphs that allow a large-scale evaluation of observed and unobserved facts.

The statistical modeling of large multi-labeled knowledge-graphs has increasingly gained attention in the recent years and its application to web-scale knowledge graphs like DBpedia, Freebase, YAGO or the recently introduced Google Knowledge Graph, has been shown. In contrast to traditional machine-learning approaches, where a mapping function on some outcome is learned based on a given fixed feature set, knowledge graph data requires a relational learning approach. In the relational learning setting generally no features are available, but the target outcome is derived from relations between entities. Due to the absence of proper features for entities, representation learning approaches and especially latent variable methods have been successfully applied to knowledge graph data. These models learn latent embeddings for entities and relation-types from the data, which provide better representations of their semantic relationships and can be interpreted as learned latent explanatory characteristics of entities. It has been shown that latent vari-

able models can successfully be exploited in tasks related to knowledge graph cleaning and completion, where they predict the uncertainty of observed and unobserved facts in the knowledge graph. Nevertheless, there has been little attention on the constraints on model complexity that arise when these models are applied to very large knowledge graphs.

1.1 Learning in the Semantic Web

Until recently, machine learning approaches in the Semantic Web domain have mainly targeted the ontologies of knowledge-bases on the schema level. In this context, the construction and management of ontologies but also ontology evaluation, ontology refinement, ontology evolution and especially ontology matching have been of major interest, where these methods generate deterministic logical statements [7, 31, 39, 71, 32, 49, 65, 64, 68]. Furthermore, machine learning approaches have been exploited for ontology learning [14, 18, 19, 108, 88, 48]. Tensors have been applied to Web analysis in [52] and for ranking predictions in the Semantic Web in [35]. An overview on mining the semantic web with learning approaches is described in [91].

1.2 Learning in Knowledge Graphs

The central learning task in knowledge graphs is link-prediction. In link-prediction the structure of the graph is learned to infer probabilities for ground triples that reflect if they are likely to be part of the graph. In other words, we try to guess if present triples are correct or if unobserved triples are likely to be true. In [104]; [82], [113] and [11] and [50] factorization approaches were proposed for this task. Furthermore, [94] applied matrix factorization for relation extraction in universal schemas. [82] introduced the RESCAL model, a third-order tensor factorization, which exploits the natural representations of triples in a third-order tensor. This model has been the target of many published works that proposed various extensions for the original approach: [55] introduced non-negative constraints, [81] presented a logistic factorization and [50] explicitly models the 2nd and 3rd order interactions. [69] proposes a weighted version to allow RESCAL to deal with missing data. The model structure of RESCAL is nowadays also often referred to as bilinear model, bilinear layer or trigram model. [99] exploits such a bilinear layer in their neural tensor network for knowledge graph completion. [36] combines a trigram and bigram model for link-prediction in knowledge graphs (TATEC) and [114] pursues a similar approach but

with a reduced trigram model that is only able to model symmetric relations. In the Google Knowledge Vault project [25] a multiway neural network architecture is exploited to predict probabilities for ground triples that serve as priors for the automatic knowledge graph construction from unstructured text. This model was shown to achieve a similar prediction quality than the neural tensor network proposed by [99] even though it is of significantly lower complexity. Furthermore, it was shown in the same work [25] that the combination of this multiway neural network with the path ranking algorithm [60] lead to significant improvements in link-prediction quality. Combining latent variable models with graph feature models has also been proposed in [79] where it decreased the required complexity of RESCAL by increasing the quality of the predictions at the same time.

In [12] the Semantic Matching Energy model (SME) is proposed, which was later refined and improved in scalability by the translational embeddings model (TransE) [9]. Entities and relation-types are represented by latent embedding vectors in these models and the score of a triple is measured in terms of a distance-based similarity measure as motivated by [74, 73]. In addition, TransE has been the target of other recent research activities. Besides aspects of the bilinear model, [114] also exploits aspects from TransE in their proposed framework for relationship modeling. [112] proposed TransH which improves TransE's capability to model reflexive one-to-many, many-to-one and many-to-many relation-types by introducing a relation-type-specific hyperplane in which the translation is performed. This work has been further extended in [67] by introducing TransR that separates representations of entities and relation-types in different spaces; The translation is performed in the relation-space. In [58], TransE has been shown to combine well with the approaches proposed in [82, 25].

Besides developing new promising model structures to drive link-prediction quality, there have also been efforts to consider prior knowledge about the data in the various models to drive link-prediction quality. In [56, 17], it was shown that the integration of prior knowledge about the domain and range of relation-types as provided by schema-based knowledge graphs enables RESCAL to model the graph with significantly lower dimensional embeddings for entities and relation-types. In addition, [56] proposed a local closed-world assumption which can be applied to approximate the domain and range of relation-types in case they are fuzzy or absent. Local closed-world assumptions are a known concept in the semantic web domain [96]. Recently, the general nature of the observed benefits from the integration of prior knowledge about relation-types into latent variable models has been analyzed in [54]. In this work, it was demonstrated that in addition to RESCAL, also

TransE, and the multiway neural network approach used in the Google Knowledge Vault project benefit to a large extent from such prior knowledge.

General methods for link-prediction also include Markov-Logic-Networks [92] which have a limited scalability and random walk algorithms like the path ranking algorithm [60].

[80] provides an extensive review on representation learning with knowledge graphs.

1.3 Contributions of this Work

In this thesis we will study latent variable models and their application to large schema-based knowledge graphs and the made contributions can be summarized as follows:

First we will compare the state of the art of latent variable models that have been proposed for semantic web data, RESCAL [82], Translational Embeddings [10] and the Neural Network exploited by Google in their Google Knowledge Vault project [25] in the context of large knowledge graphs. All three of these methods have proven to give state of the art results in the central relational learning task, link-prediction in relational graphs [83, 56, 25, 9, 17]. Even though these approaches belong to the same class of methods, they differ in many aspects, methodically and in their initial modeling assumptions.

Second, we will show that prior knowledge on the semantics of relation-types has to be exploited in these models to drive prediction quality when applied to large knowledge graphs. This prior knowledge can be extracted from the hand-curated schema of the knowledge graphs as type-constraints on relation-types, or, as an alternative, it can be derived directly from the data by a local closed-world assumption, which we propose in this work. Both kind of prior knowledge lead to significant improvements in link-prediction quality of latent variable model, but in contrast to the type-constraints, the local closed-world assumption can also be applied on relation-types where type-constraints are absent or fuzzy.

In our third contribution, we will show that besides efforts to improve the state of the art latent variable models individually, these models are well suited for ensemble solutions for link-prediction tasks. Especially the variants of these models that are of very low complexity, meaning that they exploit a low dimensional embedding space, show great complementary strengths.

In the context of link-prediction in knowledge graphs, latent variable models are traditionally used to generate confidence scores for every possible relation between entities in a knowledge graph. These confidences are exploited to apply a binary classification on

triples, which is the basis for complementing the graph with new triples. In our last contribution, we demonstrate that statistically modeled knowledge graphs can be interpreted as probabilistic databases. Probabilistic databases have a well founded theory which enables complex querying with uncertainties through rules that goes beyond querying ground triple. We will show how intrinsic features of the latent variable models can be combined with the theory of probabilistic databases to enable efficient safe querying on knowledge graphs that have been statistically modeled with latent variable models.

The afore mentioned contributions have been published in:

[58] Denis Krompaß, and Volker Tresp. Ensemble Solutions for Link-Prediction in Knowledge-Graphs. ECML-PKDD Workshop on Linked Data for Knowledge Discovery. 2015

[54] Denis Krompaß, Stephan Baier and Volker Tresp. Type-Constrained Representation Learning in Knowledge-Graphs. Proceedings of the 14th International Semantic Web Conference (ISWC). 2015

[56] Denis Krompaß, Maximilian Nickel and Volker Tresp. *Large-Scale Factorization of Type-Constrained Multi-Relational Data.* Proceedings of the International Conference on Data Science and Advanced Analytics (DSAA2014), 2014.

[57] Denis Krompaß, Maximilian Nickel and Volker Tresp. Querying Factorized Probabilistic Triple Databases. Proceedings of the 13th International Semantic Web Conference (ISWC, Best Research Paper Nominee), 2014.

This thesis is structured as follows: In the next chapter, we will give an introduction to knowledge graphs as typically present in the Linked Open Data cloud, its representation as RDF-graph and the use and structure of ontologies in these graphs. We further discuss general deficiencies of these knowledge graphs that motivate automatic approaches for data-cleansing in, or construction of knowledge-graphs. In Chapter 3 we will give a brief introduction to Representation and Relational Learning. In addition we will review three latent variable methods that have been successfully applied to knowledge graphs and represent the current state of the art in modeling knowledge graphs. Chapter 4 contains our first contribution where we study the application of these methods to large knowledge graphs in more detail. Chapter 5 will describe and motivate the integration of prior knowledge on relation-types in form of type-constraints or a local closed-world assumption into the latent variable approaches and give empirical proof that these models benefit to a large extend from such information in link-prediction tasks. Subsequent to that we will

motivate and discuss ensemble solutions based on state of the art latent variable models for link-prediction to further drive prediction quality in chapter 6. Chapter 5 holds our last contribution, where we introduce efficient probabilistic querying on knowledge-graphs that have been statistically modeled with latent variable models. Exemplified on RESCAL, we provide proof of concept for using latent variable models for answering probabilistic queries, thereby we combine intrinsic features of the model and the theory of probabilistic databases to increase efficiency. We conclude and summarize this thesis in chapter 8.

Chapter 2

Knowledge Graphs

In this chapter we will give an introduction to knowledge graphs as used in the semantic web domain, where we focus on schema-based knowledge graphs. Thereby we will cover the motivation behind knowledge graphs, their structure and range of applications. In addition we will also discuss deficiencies of currently available knowledge graphs that basically motivate the statistical modeling of them.

Knowledge graphs or graph-based knowledge bases are databases that store facts about the world as relations between entities. Entities are real-world things or objects like persons, music tracks or locations and represent the nodes in the knowledge graph. Entities can have additional attributes that further describe them, for example height, reach and weight in case of an entity that represents a box-champion. The links in the knowledge graph are defined through relation-types, which define a certain type of relationship between entities. The relation-type `friendOf` for example relates person entities with each other, where the relation-type `bornIn` relates person entities with location entities.

The content of knowledge graphs is composed of single pieces of information also referred to as facts. These facts are often stored as subject-predicate-object triples that fully define the graph, where each triple represents a relational tuple of entities. For example, the fact that Albert Einstein is born in Ulm can be represented by the triple `(Albert_Einstein, bornIn, Ulm)`, where `Albert_Einstein` and `Ulm` are the subject and object entities, respectively, and `bornIn` is the predicate relation-type. From this triple, a human can directly connect his prior knowledge with the entities and the relation-type. This prior knowledge, acquired through experience and training allows humans to understand that the fact is about a person and his birthplace. The human expert might further know that this person is a famous scientist and that Ulm is a city. If we want machines closer to the human

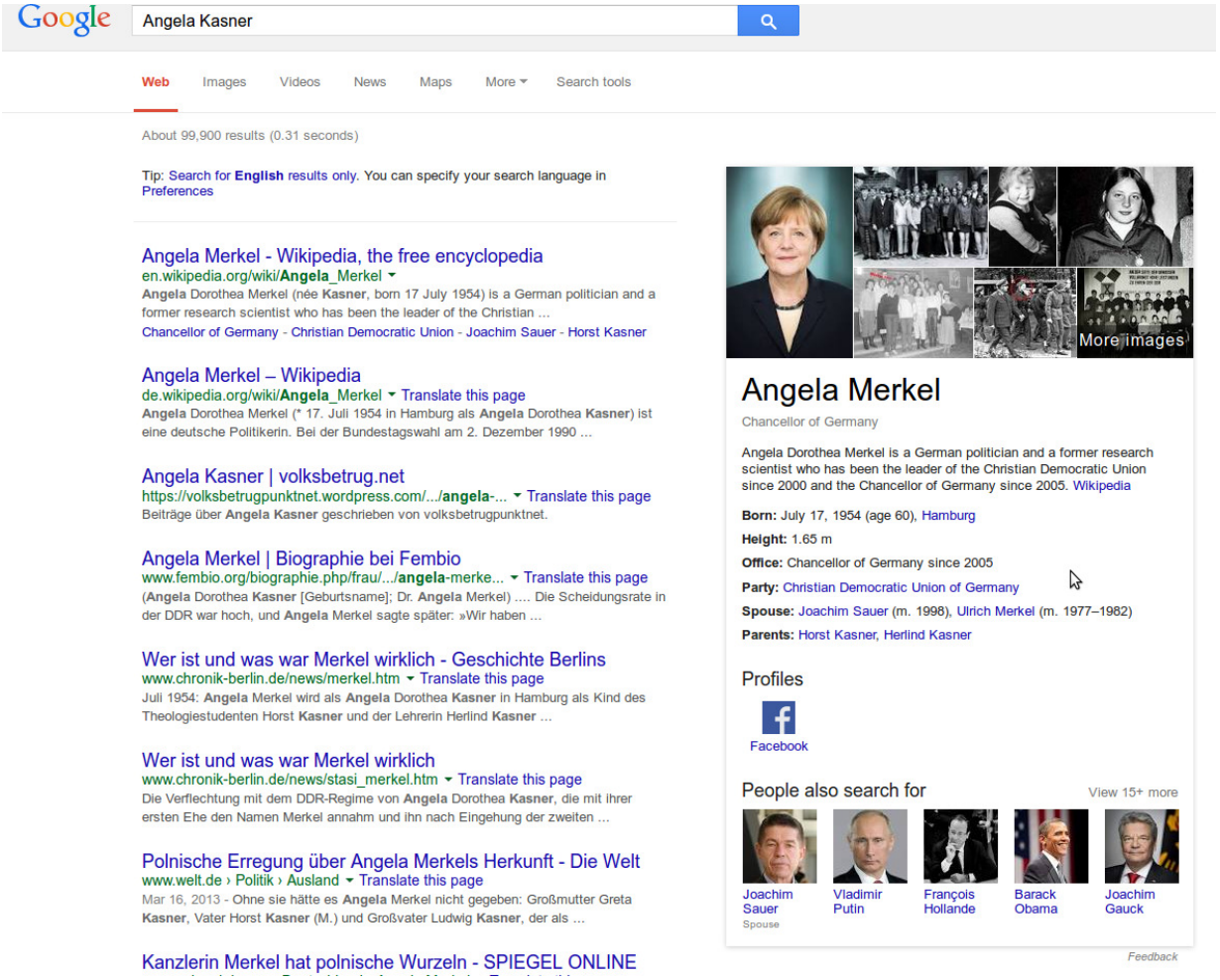


Figure 2.1: Result of Google Query “Angela Kasner”

understanding of the notion of real-world entities, we have to explicitly provide them with information that represents semantic relationships between entities. In contrast to schema-less knowledge graphs, schema-based knowledge graphs contain additional information that describe the semantics of entities and relation-types. The schema often contains an ontology for this purpose that defines e.g. class hierarchies for entities, where every entity in the graph assigned to one or several of these classes.

Referring to the previous example, we would have to represent the knowledge that the entity `Albert_Einstein` is an instance of the class `famous_scientist` and `famous_scientist` is a subclass of `person` in the knowledge graph or its schema. This kind of semantic knowledge has become very useful for areas related but not limited to search

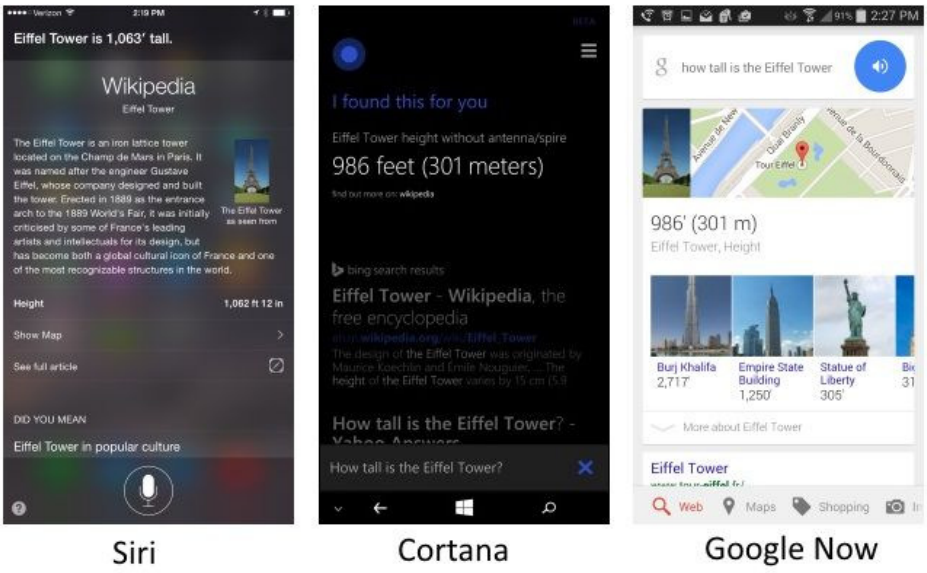


Figure 2.2: Mobile smart assistants answering the question about the height of the Eiffel Tower. Image was taken from [109]

and question answering, as successfully demonstrated by Google's search engine or IBM's Watson system. As an example, consider the question "who is the most famous scientist?". If we assume that a machine can understand that this question is about a person (e.g. through the keyword "who"), the search space can already be restricted to person entities represented in the knowledge graph.

Further, the knowledge graph can be exploited to aggregate more information than given by a query to guess on the intentions of the users. Assuming that the search query "Angela Kasner" is entered in a search application (e.g Google), the search engine will recognize that the query is about Angela Merkel, the current chancellor of Germany, since it automatically exploited information from the knowledge graph (Figure 2.1).[1] As a consequence, the combination of Angela Kasner and Angela Merkel results in highest ranked documents that are discussing the past of Angela Merkel. This can be interpreted as the attempt of the machine to guess on the intention of the user, which in this case was interpreted as the interest in getting biographic information on Angela Merkel.

In the domain of natural language processing, the information provided by knowledge graphs is exploited for word-sense disambiguation, entity resolution and relation extraction.

[1]The Google Knowledge Graph is in part powered by Freebase [8] which e.g. links "Angela Kasner" and "Angela Merkel" to the same Freebase id `m/0jl0g` by the relation-type `alias` (which is also the basis for the "Also known as" listing in Freebase entries).

Table 2.1: Abbreviations for URIs used in this work for better readability of triples.

Name-Space	Abbreviation
`http://dbpedia.org/ontology/`	`dbpo:`
`http://dbpedia.org/resource/`	`dbpr:`
`http://www.w3.org/1999/02/22-rdf-syntax-ns#`	`rdf:`
`http://www.w3.org/2000/01/rdf-schema#`	`rdfs:`

The combination of natural text extraction methods and knowledge graphs have led to very sophisticated question answering system, as impressively shown by the IBM Watson system which beat human champions in *Jeopardy!*, but also by popular smart mobile assistants e.g. Apple's *Siri*, Microsoft's *Cortana* or *Google Now* (Figure 2.2).

Today, a wide range of knowledge-graphs are available, in part domain specific as e.g. the Gene Ontology [2], but also general purpose ones like e.g. Freebase [8] or YAGO [46] that contain general knowledge partially extracted from Wikipedia, the currently biggest online encyclopedia. Freebase has been acquired by Google in 2010 and powers in part the Google Knowledge Graph [98] and the recently published Google Knowledge Vault [25]. This graph supports Google's search engine and is also exploited in various other applications developed by Google as for example *Top Charts* or *Google Now*. In addition, thanks to the effort of the linked open data initiative [6], many of these knowledge graphs have been interlinked, allowing a facilitated integration of various data sets in an application.

2.1 Knowledge-Graphs are RDF-Triplestores

Generally, graph based knowledge-bases like YAGO [46] or DBpedia [66] store their facts as triples that more or less follow the W3C Resource Description Framework (RDF) [61] standard. The RDF defines the data model for the Semantic Web. The choice to represent a labeled, directed graph through triples was driven by the goal of least possible commitment to a particular data schema, by using the simplest possible structure for representing such information. RDF allows a rich structuring of semantic web data. In this section, we will only cover the most important concepts relevant for this thesis and refer the interested reader to [44]. Further we will use the name-space abbreviations shown in Table 2.1 for better readability of triples.

2.1.1 RDF-Triple Structure

RDF-triples follow a subject-predicate-object (s, p, o) pattern, where the subject is filled through resources or blank nodes, the predicate resource represents the relationship[2] between the subject and the object entity and the object can be resources, blank nodes or literals.

Resources

In a RDF-triple, resources are represented by their Internationalized Resource Identifier (IRI), a generalization of the Uniform Resource Identifier (URI), which can be an Uniform Resource Locator (URL). Resources are the "things" in the knowledge graph like persons or locations but also abstract concepts. Throughout the rest of this thesis, we generally refer to resources that occur as subject or object in a RDF-triple if we speak of *entities*. Additionally, the term *relation-type* always refers to resources that occur as predicates in such a triple. As an example, consider the triple (`dbpr:Angela_Merkel`, `dbpo:birthPlace`, `dbpr:Hamburg`), extracted from DBpedia. In this triple, `dbpr:Angela_Merkel` is the subject entity, `dbpr:Hamburg` the object entity and `dbpo:birthPlace` the predicate relation-type that relates Angela Merkel to her birthplace Hamburg.

Literals

Literals are the direct embedding of values into the graph such as dates, strings or numbers that describe a resource. The different textual representations for the entity that represents the resource `Angela_Merkel`, "Angela Merkel" and "Angela Kasner" or the birth-date are for example literals. In difference to resources or blank nodes, literals should never occur as subjects in a triple, or in other words, literal nodes in the graph are not supposed to have any outgoing links.

Blank Nodes

Blank nodes are auxiliary nodes that do not provide any explicit content but allow the construction of e.g. higher order facts. In order to differentiate resources from blank nodes, each blank node is identified by a node identifier instead of an IRI. The node identifier is required to enable multiple resources to reference on the same blank node. Blank nodes

[2] Also often referred to as properties or relation-types.

are omitted from upcoming discussions, because they are not explicitly considered by the methods proposed and discussed in this work for knowledge graph modeling.

2.1.2 Schema Concepts

As mentioned in the introduction of this chapter, entities are generally typed in schema-based knowledge graphs, meaning that they have been assigned to predefined classes that are organized in an ontology that is part of the schema. An ontology describes a data model of the target domain of the graph including the vocabulary that describes this domain. In addition, these ontologies can be used to represent implicit knowledge by defining subclass hierarchies which can be materialized through reasoning. For example, consider all triples of the form (`<?>`, `rdf:type`, `dbpo:MusicalArtist`) present in DBpedia, where `<?>` is used as a variable for all entities that have been assigned to the class `MusicalArtist`. With an ontology that contains the subclass relationship (`dbpo:MusicalArtist`, `rdfs:subClassOf`, `dbpo:Person`), we can implicitly represent the knowledge that all entities that are musical artists are also persons.

Light-weight ontologies can be defined through the RDF-Schema (RDFS) [20] concepts, which allow the definition of classes and class hierarchies. In Table 2.3 a small section of the DBpedia ontology is represented in RDFS, the corresponding ontology is visualized below in Figure 2.3. More complex ontologies can be constructed with the Web Ontology Language (OWL) [85] but in general, more complex ontologies increase the computational costs for reasoning. When constructing ontologies, there is always a trade-off between the complexity of the defined ontology and the efficiency of the appropriate reasoner. We refer to [1] for more details on OWL.

Besides the entities that can be semantically refined through ontologies, also relation-types can be semantically described using RDFS as well. In knowledge graphs, generally two types of relation-types exist, *DatatypeProperties* and *ObjectProperties*, where the former relates entities to literals and the latter relates entities to entities. Also, relation-types can form hierarchies. In correspondence to `rdfs:subClassOf`, RDFS offers the `rdfs:subPropertyOf` concept to define hierarchies of relation-types that can be exploited by reasoners. A comprehensible example for such a hierarchy are couples that have a marriage and those that have a happy marriage. Clearly, the person entities that are related by a `happy marriage` are also implicitly related by `marriage`.

Besides enabling the definition of relation-type hierarchies, RDFS offers the concepts `rdfs:domain` and `rdfs:range` to implement *type-constraints*. These two concepts describe

Table 2.2: Defining type-constraints on the relation-type `dbpr:bandMember` using RDFS

id	Subject	Predicate	Object
1	`dbpr:bandMember`	`rdfs:domain`	`dbpo:Band`
2	`dbpr:bandMember`	`rdfs:range`	`dbpo:Person`

Table 2.3: Section extracted from the DBpedia ontology represented in RDFS. Breakdown of abbreviations can be inferred from Table 2.1

Subject	Predicate	Object
`dbpo:Artist`	`rdfs:subClassOf`	`dbpo:Person`
`dbpo:MusicalArtist_Gibbons`	`rdfs:subClassOf`	`dbpo:Artist`
`dbpo:Writer`	`rdfs:subClassOf`	`dbpo:Artist`
`dbpo:Singer`	`rdfs:subClassOf`	`dbpo:MusicalArtist`
`dbpo:MusicalDirector`	`rdfs:subClassOf`	`dbpo:MusicalArtist`
`dbpo:MusicComposer_Gibbons`	`rdfs:subClassOf`	`dbpo:Writer`
`dbpo:SongWriter`	`rdfs:subClassOf`	`dbpo:Writer`

the semantics of a relation-type by explicitly defining which entity classes should be related. Obviously, the relation-type `dbpo:birthPlace` should not be used to relate instances of the class `dbpo:Person` with each other, but persons to locations (`dbpo:Location`). In Table 2.2 type-constraints on the relation-type `dbpr:bandMember` are shown. `dbpr:bandMember` is defined to relate instances of the class `dbpo:Band` to instances of the class `dbpo:Person`.

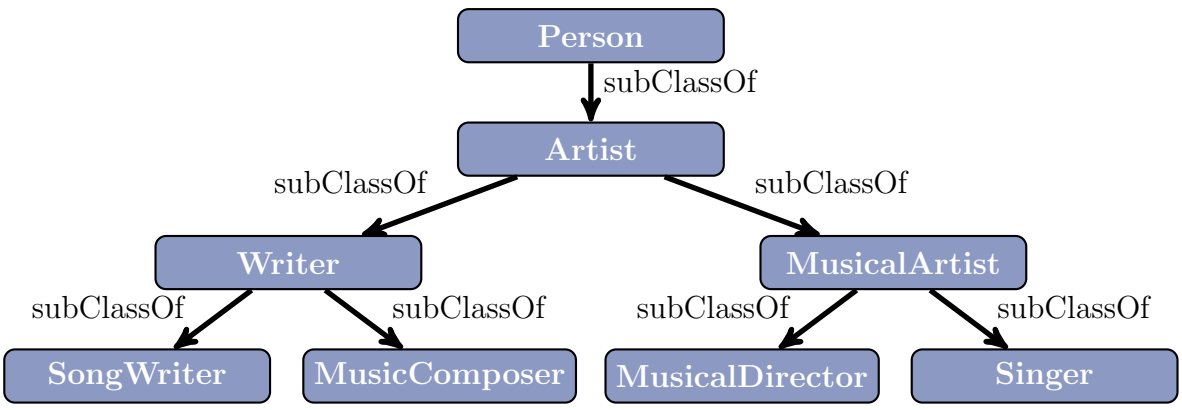


Figure 2.3: Illustration of ontology described in Table 2.3

Table 2.4: Example facts from DBpedia regarding the resources Billy Gibbons and Nickelback. The breakdown of abbreviations can be inferred from Table 2.1

id	Subject	Predicate	Object
1	dbpr:Billy_Gibbons	dbpo:associatedBand	dbpr:Nickelback
2	dbpr:Billy_Gibbons	rdf:type	dbpo:Person
3	dbpr:Nickelback	rdf:type	dbpo:Band
4	dbpr:Billy_Gibbons	dbpo:instrument	dbpr:Fender_Telecaster
5	dbpr:ZZ_Top	dbpo:bandMember	dbpr:Billy_Gibbons
6	dbpr:Billy_Gibbons	dbpo:genre	dbpr:Hard_rock
7	dbpr:Nickelback	dbpo:genre	dbpr:Hard_rock

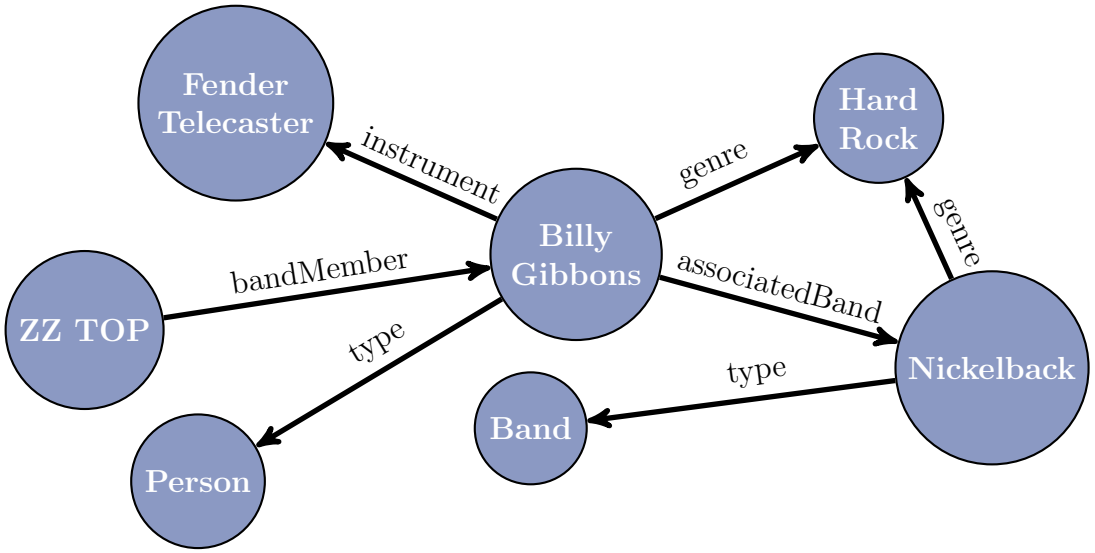


Figure 2.4: Graph representation of facts from Table 2.4

2.1.3 Knowledge Retrieval in Knowledge Graphs

As previously shown, RDF provides an easy and comprehensible way to describe and define knowledge as a graph of facts. In the following, we will show in a more concrete case how actual knowledge (and its facts) are represented and made accessible to machines.

In Table 2.4, a RDF-Triplestore consisting of 7 triples extracted from DBpedia is shown. From the first triple (`dbpr:Billy_Gibbons`, `dbpo:associatedBand`, `dbpr:Nickelback`), a human can easily understand that it describes a person named Billy Gibbons, that is somehow associated with the rock band Nickelback.[3] A human with more expertise on the band ZZ-Top could automatically connect other knowledge about Billy Gibbons as

[3]Billy Gibbons appeared on Nickelback's album *All the Right Reasons*.

e.g. that he is a guitarist of the rock band ZZ-Top. A similar principle is applied in knowledge graphs where the connections to associated information of entities are the links in the graph. Based on all facts of Table 2.4, we are able to construct a small knowledge graph (Figure 2.1.3) that can be traversed by machines, or queried, to aggregate relevant information.

RDF-structured data sets can be queried to retrieve and manipulate data. One of the most popular query languages for this task is the semantic query language SPARQL[4], which shares common principles with many other query languages such as SQL. This query language allows a user to define queries that consist of triple patterns with disjunctions and conjunctions of these patterns. The following simple example shows how SPARQL works in principle:

```
PREFIX dbpr: <http://dbpedia.org/resource/>
PREFIX dbpo: <http://dbpedia.org/ontology/>
PREFIX rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>
SELECT ?somebody
WHERE{
?somebody dbpo:instrument dbpr:Fender_Telecaster.
?somebody rdf:type dbpo:MusicalArtist.
dbpr:ZZ_Top dbpo:bandMember ?somebody.
}
```

In the top part we simply defined abbreviations for the name-spaces for better readability of the subsequent SPARQL query (`PREFIX`). In the actual SPARQL query, we ask for an entity in the database (denoted by `?somebody`) that is a musical artist (`?somebody rdf:type dbpo:MusicalArtist`) and band member of the rock band ZZ-TOP that plays a Fender Telecaster. When using the SPARQL-Endpoint[5] of DBpedia to evaluate the above query [6], the entity `dbpr:Billy_Gibbons` is returned.

2.2 Knowledge Graph Construction

In this section, we will describe how knowledge graphs are constructed in principle. Basically, knowledge graph construction can be achieved by different kinds of approaches that

[4]SPARQL Protocol and RDF Query Language.
[5]Services that process SPARQL queries.
[6]http://dbpedia.org/sparql

require different levels of human involvement. The order in which these approaches are described next approximately reflects the size of the resulting knowledge graph and the chronology in which they have been applied.

2.2.1 Curated Approaches

Curated approaches contain the earliest knowledge graphs that were mainly constructed by a small group of human experts. The first knowledge graphs for computers, originally denoted as semantic nets, were invented in 1956 for machine translation of natural languages [93]. A prominent example for a widely used knowledge graph, initially constructed by the Cognitive Science Laboratory of Princeton University, is WordNet [33]. WordNet has a central role in many applications in the natural language processing domain. From all available knowledge graphs, curated knowledge graphs are clearly the most accurate ones and complete ones. Unfortunately, due to their dependence on human experts, they are not very scalable and normally cover highly specialized domains that can be represented by small graphs.

2.2.2 Collaborative Approaches

Collaborative knowledge graph construction relies on a large community of voluntary contributors that add new facts to the knowledge graph. Additionally, the editing and quality control is also based on these contributors. Even though collaborative approaches can lead to large knowledge bases, such as Wikipedia [37] or in part the Freebase [8] knowledge graph, their scalability is always dependent on their popularity; popularity has direct impact on the size of the community of contributors. In addition, the growth of such knowledge graphs will eventually decrease, because it becomes harder for the broad community of contributors to add new triples to the graph. Besides the graph in a whole, also the contained topics are dependent on popularity and as a consequence, less popular content generally lacks extensive revision.

2.2.3 Automated Approaches on Semi-Structured Textual Data

Fully automatic construction approaches such as YAGO [46], DBpedia [66] or Freebase [8] extract their content from semi-structured sources such as tables (e.g. Wikipedia Infoboxes) and the schema (e.g. WordNet Taxonomy or the Wikipedia category system) or structured sources such as other knowledge graphs. The concepts extracted from semi-structured data

often lack proper disambiguation. For example, in Wikipedia Infoboxes a person can be related by multiple concepts to his birthplace, such as “Place of birth”, “born in” or “birthplace”, which all have the same semantics. Similarly, different ontologies used by different knowledge graphs are often not properly interlinked. These ontologies often share semantically equal entities and classes, but the mapping of entities and classes between the ontologies is often absent. To solve these issues, the extraction of facts is backed by hand-curated rules that properly resolve disambiguation. The advantage of this kind of automated approach is its scalability and the reduced amount of human involvement, leading to very accurate knowledge representations. The growth and quality of knowledge graphs that are constructed this way are not directly dependent on a large community of voluntary contributors, but on the quality of their data sources. These sources are of course dependent on a large community of contributors that provide the semi-structured data. As a consequence, these automatically constructed knowledge graphs also suffer from similar deficiencies as the collaborative constructed ones, especially incompleteness.[102]

2.2.4 Automated Approaches on Unstructured Textual Data

Due to the problems observed in the other three approaches, the main goal of the most recent research efforts is the construction or completion of knowledge graphs based on unstructured textual data. In Wikipedia, the currently largest online encyclopedia on the web, only a small fraction of its content is covered by the semi-structured infoboxes. The majority of information in Wikipedia, and generally on the Web, is contained in unstructured textual data, that is the natural language description of the articles. The NELL (Never Ending Language Learner) project [16] tries to “read the web” to extract new facts from unstructured textual web content. Recently, [25] proposed an approach where the statistical modeling of existing knowledge graphs (Freebase) can be combined with relation extractors applied on unstructured text documents to complement the content of these knowledge graphs accurately on a large scale. The principle of this approach is illustrated in Figure (2.5). In the first step, a text extraction tool is applied on textual data for triple extraction, which additionally provides a measure of confidence (a probability) that represents the belief of the extractor that this relation is true. In parallel, the confidence of statistical models which have been applied to the knowledge graph data is retrieved for the same triple. These statistical models can be latent variable models, which are in the focus of this thesis, but also graph feature models (e.g. path ranking algorithm) are exploited for this task ([25] used a combination of both). For the final decision on which triples are

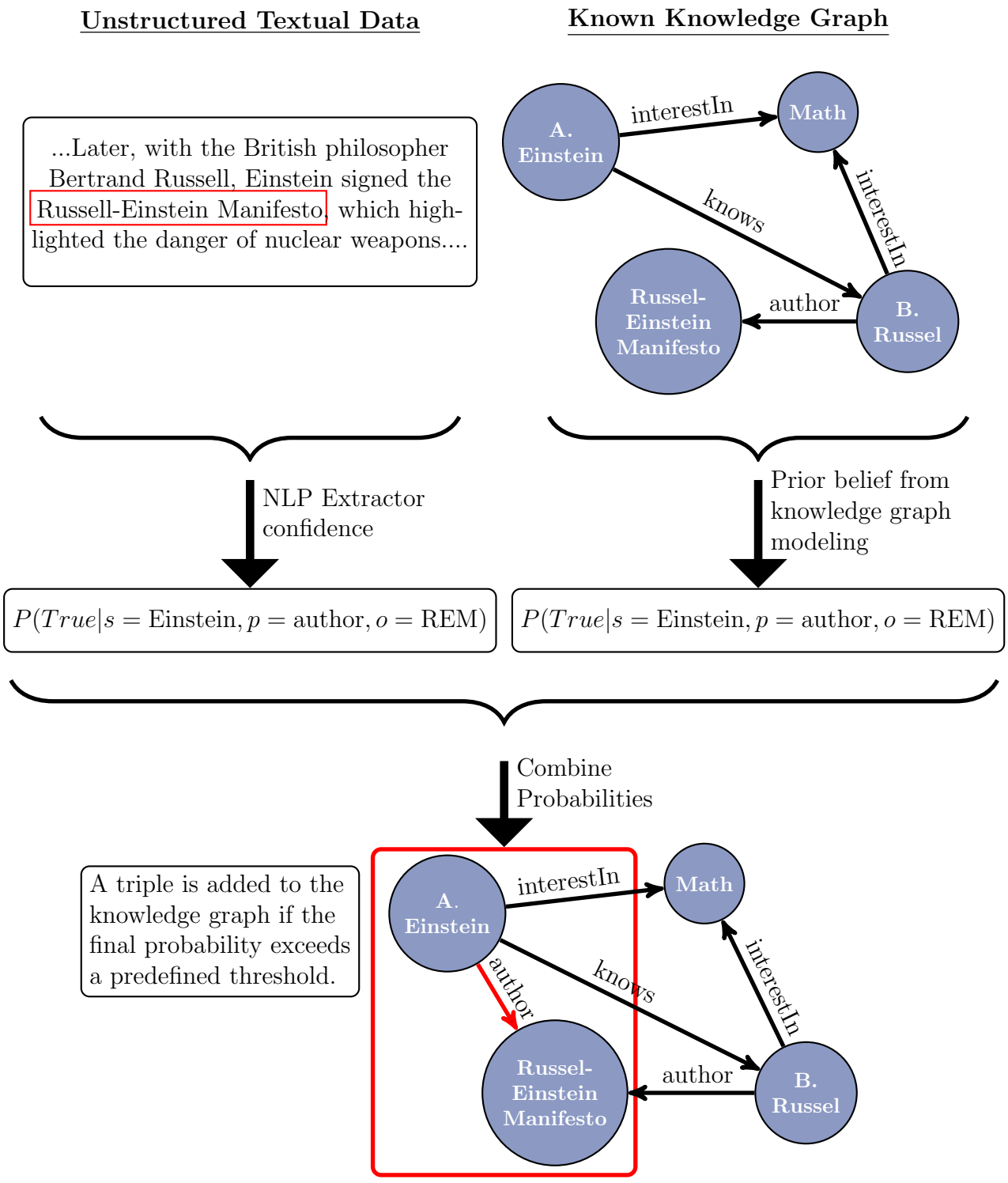


Figure 2.5: Illustration of the principle behind automatic knowledge base completion based on unstructured textual data as proposed by [25]. *REM* abbreviates Russel-Einstein Manifesto. Text was extracted from http://en.wikipedia.org/wiki/Albert_Einstein.

added to the graph, the confidences provided by the various methods are combined. It was shown in [25] that this approach significantly increased the accuracy of relation extraction from natural language text.

2.3 Popular Knowledge Graphs

In this part we will describe three widely used knowledge graphs in more detail that were also the primary source of data of the experiments conducted in this thesis, namely DBpedia [66], Freebase [8] and YAGO [46]. All of these knowledge graphs heavily rely on data from Wikipedia and are part of the Linked Open Data (LOD) cloud, an initiative that aims for the goal of interlink various open RDF-structured data sets on the web [6]. The Wikipedia online encyclopedia is with no doubt one of the most widely used source of knowledge in the Internet today. Its content is maintained by thousands of contributors and used by millions of people daily. Even though Wikipedia contains a lot of information, its search and querying capabilities are limited to find whole articles. For example, it is difficult to find all mountains above a certain height in the German alps. As already discussed in this chapter, these kind of queries can be easily answered by knowledge graphs, because they contain structured content.

2.3.1 DBpedia

The DBpedia [66] community project was started in 2006 with the goal to create a structured representation of Wikipedia that follows the Semantic-Web standards. DBpedia serves as a machine accessible knowledge graph that enables complex querying on data from Wikipedia. Besides the natural language content, Wikipedia articles are often enriched in structured information such as Infobox templates, article categorizations, geo-coordinates and links to other online-resources. Hereby, Wikipedia Infoboxes are the most valuable source of information for DBpedia, because their purpose is to list the most relevant facts of the corresponding article (especially for famous people or organizations). DBpedia provides an automatic extraction framework to retrieve facts from Wikipedia articles and stores them in a RDF-Triplestore. Here, the heterogeneity in the Wikipedia Infobox system has been a problem, because the authors did not follow one standard structure, but used different Infoboxes for the same type of entity or different relation-type names for semantically equal relationships.

A big step forward in terms of data quality could be achieved in 2010, when a community

effort has been initiated to homogenize and disambiguate the description of information in DBpedia. Through this effort, an ontology schema has been developed and the alignment between Wikipedia Infoboxes and this ontology has been leveraged by community-provided mappings that disambiguate relation-types, entities and classes. Besides disambiguation, these mappings also include the typing of resources and specific data-types for literals. In absence of those mappings, the resources extracted from the Infoboxes are saved as literal values, because their semantics are unclear to the extractor. However, even though data quality is improving, it is unlikely that DBpedia will reach the quality of manually curated data sets. In the current release (DBpedia2014), the DBpedia ontology consists of 658 classes which are related by 2,795 different relation-types. These 658 classes count 4,233,000 instances, of which 735,000 are places, 1,450,000 persons and 241,000 organizations. In total, the English version of DBpedia contains 583 million facts, but multilingual DBpedia (129 languages are included) counts approximately 3 billion RDF-triples. In addition, DBpedia provides a large amount of links to external data sets on instance and schema level.

DBpedia has become a central hub of the Linked Open Data cloud and numerous applications, algorithms and tools are using its content. In addition, DBpedia provides different types of data sets for various purposes. One example is the Lexicalization data set which is especially useful in NLP related tasks. This data set contains alternative names for entities and properties together with several measures that indicate observed frequency of the ambiguity of terms.

2.3.2 Freebase

Similar to DBpedia, Freebase [8] is also a RDF-based graph database, but in contrast to DBpedia, Freebase does not solely rely on structured information extracted from Wikipedia Infoboxes. Freebase also integrates information from many other external databases, for example MusicBrainz, WordNet and many more. In addition, facts are directly added and reviewed by a large community of voluntary contributors. This is a big difference to DBpdia, where data could only be changed by editing the corresponding Wikipedia article.

In Freebase, real world things or concepts are termed as *topics*, where each topic has an article on Freebase. Not all entities in Freebase are topics, there also exist literals that relate specific values to the topics. In addition, blank nodes are used to represent more complex facts. Similar to DBpedia, Freebase also contains *ObjectProperties* and *DatatypeProperties*. The former relation-types relate topics to entities that are no literals and the latter relate

topics to (typed) literals. In Freebase, relation-types have type-constraints, which are denoted as expected types that correspond to the rdfs:range and rdfs:domain constraints.

The Freebase ontology (called Schema) does not represent an inheritance hierarchy, but groups entity types into domains, which can also be edited by the community using an online interface.

Currently, Freebase consists of 47 million topics, 70,000 relation-types and 2.7 billion facts about them. In 2010, Freebase (Metaweb) was acquired by Google and now powers in part Google's Knowledge Graph [98] and the recently published Google Knowledge Vault [25]. In 2014, Google announced a retirement of Freebase in mid 2015 and that it will be integrated in Wikimedia-Foundation's Wikidata project [110].

2.3.3 YAGO

YAGO (Yet Another Great Ontology) is an automatically generated high quality knowledge graph that combines the information richness of Wikipedia Infoboxes and Wikipedia's category system with the clean taxonomy of WordNet. The YAGO project is basically motivated by two observations: First, Wikipedia offers a very broad view on the knowledge of the world, but its category system is not well suited as an ontology. Second, WordNet offers a very clean and natural ontology of concepts, but falls short in describing real world entities like authors, musicians etc. YAGO maps the Wikipedia categories on the WordNet ontology with a precision of 95%, thereby successfully linking these two sources of information. The YAGO entities are assigned to more than 350,000 different classes and all relations in YAGO are attached with a confidence value. It further defines a simple model, the YAGO model, that extends RDFS to allow the representation of n-ary relations, but which in contrast to complexer ontology languages, such as OWL-Full, is still decidable. The n-ary relations are realized by introducing fact identifiers that can easily be integrated in RDF. These identifiers represent blank nodes in the graph that refer to whole facts, which in turn can be used as reference in other facts to realize n-ary relations. As an example, the fact

`Albert_Einstein hasWonPrize Nobel_Prize_in_Physics inYear 1921`

can be represented by determining the core fact and assigning an identifier to it

`#1: Albert_Einstein hasWonPize Nobel_Prize_in_Physics`

and using this identifier as reference for the second fact

`#2: #1 inYear 1921`

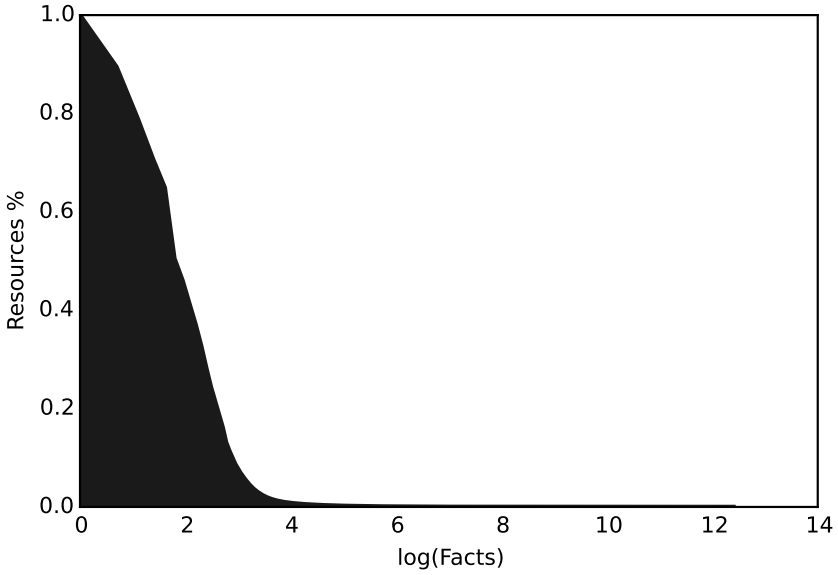


Figure 2.6: Distribution of facts per entity in DBpedia on a log scale.

In its current version (YAGO2), YAGO contains more than 10 million entities and about 120 million facts about them. In the upcoming version (YAGO3), the knowledge graph will be combined with information from multilingual Wikipedia.

In contrast to DBpedia, which basically constructs a RDF representation of Wikipedia's Infoboxes, YAGO extracts only a small number of the relation-types and corresponding relations to guarantee consistency and high precision of the knowledge-graph.

2.4 Deficiencies in Today's Knowledge Graph Data

As already mentioned in the introduction of this work, knowledge graphs generally suffer from incompleteness and inconsistencies in their data.

In terms of inconsistencies, it can be expected that the majority of contributions are correct, but nevertheless errors caused by misunderstanding of the schema, due to general carelessness or by false contributions are not rare.

The magnitude of incompleteness in these graphs can be illustrated by the following facts regarding very popular DBpedia and Freebase knowledge graphs. In English DBpedia[7], 66% of the entities typed as persons are missing a place of birth and 58% of the scientist do not have a fact that describes what they are known for. In addition, 40% of

[7]DBpedia2014, mapping-based properties (cleaned)

all countries miss a capital and 80% of the capitals do not have a leader. Even 2% of the entities are not assigned to any class. In Freebase, 71% of persons are missing a place of birth and 75% do not have a nationality [25]. Generally, it can be expected that the amount of missing information is even higher for less popular entities and relation-types.

Besides missing information, the amount of triples for each entity also varies to a large extent in the knowledge graphs, as shown in Figure 2.6 for DBpedia. It can be observed that the distribution is heavy-tailed (note the log scale) and only a minority of about 16,000 out of 4.5 million entities in DBpdia takes part in more than 100 facts (triples). However, this small fraction of entities (0.34%) occurs in 18.7% of all facts. About 50% of all entities occur in less than or equal to 5 facts and 500,000 (11%) have only one fact. It can be concluded that the vast majority of entities in DBpedia is not well described, while in contrast a large amount of information is available for a very small fraction of entities.

The reasons for this incompleteness are manifold, but the major cause lies in the fact that most of the information available today is contained in natural text documents which is hard to extract. It is certain that it is intractable for the community of voluntary contributors to structure this data manually, even a reliable quality control for all facts stored in knowledge graphs has become unreachable.

Today, growth and quality of knowledge graphs is still highly dependent on the various communities of voluntary contributors. Recently, it has been observed that the growth of Wikipedia, which serves as a central knowledge repository for many knowledge graphs, has eventually plateaued [101]. There are multiple explanations for this observation, for instance that due to the size of the database and the large community of contributors the internal bureaucracy has increased. Nevertheless, one of the main reasons lies in the fact that the amount of opportunities to contribute knowledge for the broad majority of the community decreases with the size of the database. This fact also reflects the observation that in Wikipedia a decline in editor and page growth was observed [101].

To tackle the deficiencies observed in available knowledge graphs, automatic approaches that support quality control in knowledge graphs, and boost the growth and increase completeness are in great need. In Section 2.2.4, approaches are described that tackle the relation mining from unstructured textual data sources by exploiting statistical models for knowledge graphs. These models are capable of evaluating triple quality in knowledge graphs, which can be exploited for completion and cleansing tasks for such graphs. Latent variable models have been successfully exploited for the statistical modeling of knowledge graphs and it was shown that these models scale to web-scale data sets.

Chapter 3

Representation Learning in Knowledge Graphs

In this chapter, we will cover the basics of representation learning in knowledge graphs. First, we will give a brief introduction to representation and relational learning, before we will discuss three representation learning algorithms in more detail that have been applied to knowledge graph data, namely RESCAL [82], Translational Embeddings [9] and the neural network approach used in the recent Google Knowledge Vault project [25].

3.1 Representation Learning

Generally, the predictive modeling capabilities of machine learning algorithms rely on the quality of the data that define the problem context. Here, quality refers to different important aspects that can be considered in different ways by these models: First, the noise in the data. Machine learning algorithms are data driven models, therefore it is not surprising that it is harder for them to detect dependencies and patterns in noisy data since noise can distort and mask important signals and correlations. Noise in the data is present in every real-world data set such as e.g. data recorded by sensor measurements of machines used in an industrial production environment. Reasons for noise in the data can be manifold and its removal is often connected to a trade-off between noise reduction and signal loss. In machine learning, robust and generalizing models on noisy data can be trained by applying regularization on the model parameters during training.

Second, the capability of the features present in the data to sufficiently explain the distribution of the target variables of the problem task to solve. Obviously, to recognize

if the recorded data contains enough information to model a problem task can be very challenging. There might be confounding factors that are not recorded in the data, but have a dramatic impact on the target outcome. Dependent on the importance of the confounding factors for the modeling, a learning task can become infeasible. In a less dramatic case, but still very challenging, the recorded factors (features) contain enough information to reason on the target distribution, but correlations are hidden or not obvious enough to be easily recognized by the learning algorithm. As a simple example, consider a lung cancer risk prediction task where no information about the patient's smoking habits are included in the data (e.g. if the patient is a smoker and how many cigarettes are consumed every day). It is generally known that there is a strong correlation between smoking and lung cancer risk. However, in the latter case there might be other features present in the data from which we could conclude on the smoking habits of a patient (e.g. a combination of age, teeth color, blood pressure, blood sodium level etc.), which themselves do not have an obvious correlation with lung cancer. Traditional machine learning methods have problems to extract and organize such discriminative information from the data. In this situation, feature engineering can often be applied to manually or semi-automatically construct additional features that incorporate human prior (expert) knowledge which explain the target variables more obvious to the learning algorithm. For the previous example we would introduce a "smoker" feature in the data that is derived from the other features by a human expert or through some given formula exploited as basis function. Unfortunately, feature engineering has the disadvantages that it can be quite labor-intensive and often domain experts have to be consulted for suitable feature construction (e.g. in the lung cancer risk prediction example we would need physicians that are familiar with clinical traits of smokers).

Representation Learning, often also referred to as feature learning, proposes a different approach that avoids the dependence on labor extensive feature engineering, but tries to automatically discover good latent features that disentangle hidden correlation present in the data. However, in difference to the raw input or hand engineered features which most often have a clear interpretation, these learned latent features are often hard to interpret. In Representation Learning a transformation of the raw input data into a new latent feature space is learned, where this feature space consists of explanatory factors that are more useful for a classifier or other predictor. Even though this latent feature space is a better basis for the learning task to solve than the feature space spanned by the original raw features, this does not mean that it has to be more complex. In fact, the opposite is

often the case since raw data often contains redundant dependencies or large amounts of other dispensable information that is not necessary for representing the underlying data generating function. Tensor/matrix factorization or Autoencoders are typical approaches where the latent feature space is enforced to be much smaller than the original feature space in order to learn the most general factors that are important to explain the distribution of the data. [45, 41, 105, 51]

Expressive new representation of input data can be learned in a supervised or unsupervised setting. In the supervised setting, the new representations are directly learned with respect to the given labels from the supervised task, thereby leading to latent factors that disentangle correlations to the target variable. This approach is often executed with neural networks, where the first layer is responsible for learning the first raw feature transformation which is combined to generate the final output, or in case of deep networks (e.g. convolutional neural networks for image recognition), to form the input for further feature transformations to realize complex latent representation hierarchies.

Learning good representations for a target task can be difficult if the amount of labeled training data falls short in comparison to the complexity of the learning problem. Good representations can also be learned in an unsupervised settings and exploited, if desired, in a supervised learning task as a fixed input data transformation or as initialization for the representation layer in a neural network. It is often convenient to assume that representations that explain much of the distribution of the input data tend to also explain much of the target distribution. In addition, generally plenty of data for a unsupervised learning scenario is available or can be collected very easily. As an example, consider a document topic classificator which exploits latent representations of words. Intuitively, we would directly assume that the topic of a document is dependent on the distribution of words in a document and therefore learning representations that explain the distribution of words in a document, independent from the topic, should be beneficial for the topic classification. In difference to the topic learning task, where only a limited amount of labeled training data is available, for the unsupervised learning task that tries to learn good representations of words that explain the distribution of words in documents, almost unlimited amounts of training data is available.[28, 86]

Probably the best known representation learning approach is the Singular Value Decomposition (SVD), which is also exploited in the Principal Component Analysis (PCA) and learns latent factors that explain most of the variance observed in the data. Non-negative matrix factorization has been exploited in text or image processing [59, 63] where

in case of the images, the latent factors could be interpreted as local structures like eyes, ears or noses. Factorization Machines [89] have been quite successful in recommendation settings, learning latent representations for users and items. Higher order tensor factorization methods were used on various data set such as EEG data where the latent factors have been exploited to analyze epileptic seizures [76]. Tensor factorization has also been exploited in image processing tasks e.g. for Tensor Faces [107], a generalization of Eigenfaces [106], that additionally considers various perspectives of face images as additional modes in the tensor.

More recently, deep learning approaches have gained much popularity and have been applied in a variety of fields, including speech recognition and signal processing, object recognition, natural language processing (NLP) and multi-task learning, often representing the current state of the art with leading performance on various benchmark sets [22, 53, 72]. The representations learned by these models, as for example in convolutional neural networks in the context of images, have even outperformed approaches that exploited sophisticated feature engineering through human experts. We refer to [4] for a very good review on representation learning with deep architectures at this point.

In difference to the various types of data representation learning has been applied to, with knowledge graphs we are dealing with graph structured data where the nodes are defined through their connections in the graph and not solely on a fixed set of features that describe them. Similar to the word setting in NLP, the raw data is often purely symbolic, meaning that we have just the URI of the entity (or words in the NLP setting) and the context this symbol appears in without any features that describe the characteristics of the entity. Having expressive distributed representations of entities that contain the general explanatory factors for the dependencies observed in the graph makes these symbolic URIs comparable, meaning that similar entities that share a similar representation should have similar connections in the graph. In a sense, the goal of representation learning in knowledge graphs is to disentangle the semantics of entities solely based on the observed relationships between entities in the graph. Learning from these relationships is referred to as *Relational Learning* which we will discuss in the next section.

3.2 Relational Learning

In (traditional) non-relational learning settings, the data consist mainly of features that describe measured characteristics of instances (or entities), as for example in an arbitrary

population study that collects attributes like size, age, gender, employee, academic degree etc. of different persons. Generally when dealing with this kind of data sets, independence between these instances is assumed to simplify the learning problem. As a consequence, the learning algorithm will only model dependencies between the given features and some target variable we want to predict. For example, consider the learning problem where we want to predict the income of persons based on the schematically described data set from the previously mentioned population study. In this case, the learner will predict the income for each person individually without considering any dependence on the other persons in the data set.

In a relational learning setting we eventually discard this strict independence assumption by exploiting data that explicitly reflects dependencies between the instances in the learning algorithms. Referring to the previous example, we might also know which of the persons in the data are friends or work in the same company. Assuming dependencies between entities in the data generally increases the complexity of the learning problem, which can become intractable. Today's relational learning algorithms have managed to decrease complexity to a manageable size allowing an application on even very large data sets.

There are dependency patterns that are present in relational data that can be exploited by relational learning algorithms, but not by non-relational learners [78]. In relational data, it is often observed that entities with similar characteristics are related to each other. This observation is termed *homophily* and is exploited for predicting relations between similar entities, but also to predict attributes. As an example, persons with the same age, income and academic background might be employed at the same company. Further, if they work in the same company, they might even know each other or are even friends. *Stochastic equivalence* on the other hand describes the observation that similar entities form groups and that the relationships observed in the graph can be explained by the relationships of these groups. This dependency can be exploited for clustering of entities, but also for predicting new relationships, since the members of one group tend to have similar relationships to members of other groups. Additionally, the relational data might contain *global dependencies*, which can be understood as (complex) rules that can be exploited by the learning algorithm. For example, actors that played in movies with high ratings are probably rich.

The exploitation of these dependencies, which are also present in graph based knowledge representations, make relational learning algorithms especially attractive for applications

in knowledge graphs. There exist a wide range of relational learning algorithms and in this work we only consider statistical relational learning methods, which model statistical dependencies observed in the knowledge graph. More specific, we focus on latent variable methods that learn distributed representations for entities and relation-types and have been successfully applied to the relational domain. The main application of these methods in knowledge graphs is *link-prediction*, meaning that the learning algorithms propose new relations between existing entities that can be added to the graph to enrich its knowledge content. Link-prediction is the basis for tasks related to knowledge graph cleansing and completion and plays a central role in automatic knowledge graph construction methods based on unstructured textual information (see Chapter 2.2.4). Further, the learned distributed representations of entities can be exploited for *link-based clustering*, but also for *entity resolution*, often used in tasks related to the disambiguation of entities. For the interested reader, we refer to [80] for an extensive review on relational learning in knowledge graphs.

3.3 Statistical Modeling of Knowledge Graphs with Latent Variable Models

In the following we will briefly review the latent variable models RESCAL, TransE and the neural network approach used in the recent Google Knowledge Vault project [25] (denoted as multiway neural network (mwNN) in the following) in more detail. We selected these models for a number of reasons:

- To the best of our knowledge, these latent variable models are the only ones which have been applied to large knowledge graphs with more than 1 million entities, thereby proving their scalability [9, 25, 83, 17, 56].

- All of these models have been published at well respected conferences and have been the basis for the most recent research activities in the field of statistical modeling of knowledge graphs (see the related work in Chapter 4.4).

- These models are very diverse, meaning they are very different in the way they model knowledge graphs. These differences cover a wide range of possible ways a knowledge graph can be statistically modeled; the RESCAL tensor-factorization is a bilinear model, whereas the distance based TransE models triples as linear translations and

mwNN exploits non-linear interactions of latent embeddings in its neural network layers. Further, RESCAL uses a Gaussian likelihood function that can be minimized very efficiently via ALS, but as a drawback it has to exploit closed-world assumptions[1]. Knowledge graphs are generally not containing any negative evidence and therefore considering all unobserved triples as missing instead of false seems more appropriate. TransE exploits a margin bases ranking loss function that better integrates the notion of missing triples. Nevertheless, in some cases it can be argued that many triples can be treated as negative evidence. In [25] it is assumed that if a subject predicate pair s,p is observed in the data, than all possible triples (s,p,$\cdot$), where $\cdot$ can be substituted by any entity observed in the data, are either positive (if observed in the data) or negative evidence. This assumption is motivated by the observation that if triples for a subject predicate pair are added to the graph, they are fairly complete and most unobserved triples will be very likely false. In this case, it can make sense to minimize a Bernoulli likelihood loss function as done by the mwNN model.

We belief that because of the reasons above, these models are well suited to show the generality of the contributions of this thesis for the application of latent variable models in the context of large knowledge graphs.

3.3.1 Notation

In the following, $\underline{\mathbf{X}}$ will denote a three-way tensor, where $\mathbf{X}_k$ represents the k-th frontal slice of the tensor $\underline{\mathbf{X}}$. $\mathbf{X}$ or $\mathbf{A}$ denote matrices and $\mathbf{x}_i$ is the i-th col vector of $\mathbf{X}$. A single entry of $\underline{\mathbf{X}}$ will be denoted as $x_{i,j,k}$. Further *(s,p,o)* will denote a triple with subject entity s, object entity o and predicate relation-type p, where the entities s and o represent nodes in knowledge graph that are linked by the predicate relation-type p. The entities belong to the set of all observed entities $\mathcal{E}$ in the data.

3.3.2 RESCAL

RESCAL [82] is a three-way-tensor factorization model that has been shown to lead to very good results in various canonical relational learning tasks like link-prediction, entity resolution and collective classification [83]. One main feature of RESCAL is that it can exploit a collective learning effect when used on relational data, since an entity has a unique

[1] All combinations of triples that are not observed in the graph are treated as negative evidence.

representation over occurrences as a subject or as an object in a relationship and also over all relation-types in the data. When dealing with semantic web data, multi-relational data is represented as triples that have a natural representation in a third-order adjacency tensor $\underline{\mathbf{X}}$ of shape $n \times n \times m$, where n is the amount of observed entities in the data and m is the amount of relation-types. Each of the m frontal slices $\mathbf{X}_k$ of $\underline{\mathbf{X}}$ represents an adjacency matrix for all entities in the data set with respect to the k-th relation-type.

Given the adjacency tensor $\underline{\mathbf{X}}$, RESCAL computes a rank d factorization, where each entity is represented via a d-dimensional vector that is stored in the factor matrix $\mathbf{A} \in \mathbb{R}^{n \times d}$ and each relation-type is represented via a frontal slice $\mathbf{R}_k \in \mathbb{R}^{d \times d}$ of the core tensor $\underline{\mathbf{R}}$, which encodes the asymmetric interactions between subject and object entities. The embeddings are learned by minimizing the regularized least-squares function

$$\mathcal{L}_{RESCAL} = \sum_{k}^{m} \|\mathbf{X}_k - \mathbf{A}\mathbf{R}_k\mathbf{A}^T\|_F^2 + \lambda_A\|\mathbf{A}\|_F^2 + \lambda_R \sum_{k}^{m} \|\mathbf{R}_k\|_F^2 \ , \tag{3.1}$$

where $\lambda_A \geq 0$ and $\lambda_R \geq 0$ are hyper-parameters and $\|\cdot\|_F$ is the Frobenius norm. The cost function can be minimized via very efficient Alternating-Least-Squares (ALS) that effectively exploits data sparsity [82] and closed-form solutions. During factorization, RESCAL finds a unique latent representation for each entity that is shared between all relation-types in the data set.

The confidence score $\theta_{s,p,o}$ of a triple (s, p, o) is predicted by RESCAL through reconstruction by a vector-matrix-vector product

$$\theta_{s,p,o} = \mathbf{a}_s^T \mathbf{R}_p \mathbf{a}_o \tag{3.2}$$

from the latent representations of the subject and object entities $\mathbf{a}_s$ and $\mathbf{a}_o$, respectively, and the latent representation of the predicate relation-type $\mathbf{R}_p$.

3.3.3 Translational Embeddings

In [9] a distance-based model was proposed for learning low-dimensional embeddings of entities (TransE), where relationships are represented as translations in the embedding space. The approach assumes for a true triple that a relation-type specific translation function exists that is able to map (or translate) the latent vector representation of the subject entity to the latent representation the object entity. The confidence of a fact is expressed by the similarity of the translation from subject embedding to the object

embedding.

In case of TransE, the translation function is defined by a simple addition of the latent vector representations of the subject entity $\mathbf{a}_s$ and the predicate relation-type $\mathbf{r}_p$. The similarity of the translation and the object embedding is measured by the L_1 or L_2 distance. TransE's confidence $\theta_{s,p,o}$ in a triple (s, p, o) is derived by

$$\theta_{s,p,o} = -\delta(\mathbf{a}_s + \mathbf{r}_p, \mathbf{a}_o), \tag{3.3}$$

where δ is the L_1 or the L_2 distance and $\mathbf{a}_o$ is the latent embedding for the object entity. The embeddings are learned by minimizing the margin-based ranking cost function

$$\begin{aligned} \mathcal{L}_{TransE} &= \sum_{(s,p,o)\in T} \mathbf{max}\{0, \gamma + \theta_{s',p,o} - \theta_{s,p,o}\} + \mathbf{max}\{0, \gamma + \theta_{s,p,o'} - \theta_{s,p,o}\} \\ \text{with} \quad & \{s', o'\} \in \mathcal{E} \end{aligned} \tag{3.4}$$

on a set of observed training triples T through Stochastic Gradient Descent (SGD), where $\gamma > 0$ is the margin and the corrupted entities s' and o' are drawn from the set of all observed entities $\mathcal{E}$. Note that subject and object entities are never replaced at the same time. Instead, for one triple out of T two corrupted ones are sampled where either the subject or the object entity is replaced by a random entity. During training, it is enforced that the latent embeddings of entities have an L_2 norm of 1 after each SGD iteration.

3.3.4 Google Knowledge-Vault Neural-Network

The Google Knowledge Vault project [25] pursues an automatic construction of a high quality knowledge graph. In this regard a multiway neural network (mwNN) based model for predicting prior probabilities for triples from existing knowledge graph data was proposed to support triple extraction from unstructured web documents. The confidence value $\theta_{s,p,o}$ for a target triple (s, p, o) is predicted by

$$\theta_{s,p,o} = \sigma(\beta^T \phi\left(\mathbf{W}\left[\mathbf{a}_s, \mathbf{r}_p, \mathbf{a}_o\right]\right)) \tag{3.5}$$

where $\phi()$ is a nonlinear function like e.g. *tanh*, $\mathbf{a}_s$ and $\mathbf{a}_o$ describe the latent embedding vectors for the subject and object entities and $\mathbf{r}_p$ is the latent embedding vector for the predicate relation-type p. $[\mathbf{a}_s, \mathbf{r}_p, \mathbf{a}_o] \in \mathbb{R}^{3d\times 1}$ is a column vector that stacks the three embeddings on top of each other. $\mathbf{W}$ and β are neural network weights and $\sigma()$ denotes

the sigmoid function. The model is trained by minimizing the Bernoulli cost-function

$$\mathcal{L}_{mwNN} = -\sum_{(s,p,o)\in T} \log \theta_{s,p,o} - \sum_{o'\in\mathcal{E}}^{c} \log(1-\theta_{s,p,o'}) \tag{3.6}$$

through SGD, where c denotes the number of corrupted triples sampled under a local closed-world assumption as defined by [25], where only the object entity is corrupted by a random entity drawn from $\mathcal{E}$. Note that we only sample observed triples (which are assumed to be true) and the corrupted triples generated from these are all treated as negative evidence.

Chapter 4

Applying Latent Variable Models to Large Knowledge Graphs

In this chapter we study the different latent variable models introduced in Chapter 3.3 with regard to their application to large knowledge graphs. Due to their size, large knowledge graphs require to constrain the complexity of the latent embeddings for entities and relation-types exploited by these models. These constraints are mostly disregarded in the discussions and conclusions of related literature, but are very important to consider when selecting and applying these models to large data sets. In the following sections we will give more details to these constraints and describe their impact on TransE, RESCAL and mwNN. We further simulate the application of these models (link-prediction) on large knowledge graphs based on various data sets, in order evaluate their performance in such a setting.

Own contributions in this chapter are part of our prior work on the contributions described in Chapter 5. The experimental results regarding the area under precision recall curve (AUPRC) and area under receiver characteristic (AUROC) scores shown in Tables 4.3, 4.4 and 4.5 have been published in

[54] Denis Krompaß, Stephan Baier and Volker Tresp. Type-Constrained Representation Learning in Knowledge-Graphs. 14th International Semantic Web Conference (ISWC). 2015

Table 4.1: Parameter complexity of models regarded in this work, where n is the amount of entities and m the number of relation-types present in the data. d denotes the size of the latent space or rank of the factorization and l is the number of hidden units in the second layer of the *mwNN* model.

Model	Parameter Complexity
RESCAL	$\mathcal{O}(nd + md^2)$
TransE	$\mathcal{O}(nd + md)$
mwNN	$\mathcal{O}(nd + md + ld + l)$

4.1 Latent Variable Model Complexity in Large Knowledge Graphs

When comparing the RESCAL, TransE and mwNN latent variable models based on their parametrization complexity shown in Table 4.1, RESCAL has clearly the highest complexity, because it scales quadratic with the chosen embeddings dimension d and the amount of relation-types m present in the data. TransE on the other hand has the most parsimonious parametrization followed by the mwNN model, which both scale linearly with respect to the chosen dimensionality d of the embeddings. In addition to the other models, mwNN has an additional parameters of size l present in the hidden neural network layers. When dealing with large knowledge graphs, these differences in parameter complexity between RESCAL, TransE and mwNN become negligible for the following two reasons:

- Generally, knowledge graphs contain millions of entities, but the amount of relations types is only in the thousands. Therefore, the complexity of nd, which depends on the amount n of entities observed present in the knowledge graph and the chosen dimensionality d of the latent embeddings, will dominate the parameter complexity in all three models.

- For the statistical modeling of large knowledge graphs the latent embeddings have to be meaningful in low dimensional latent spaces; higher dimensionality can cause unacceptable runtime performances and high memory loads.

It can be concluded from these two reasons that the choice of a tractable dimensionality for the latent embeddings is mostly dependent on the number of nodes (entities) in the graphs. As a consequence, these algorithms cannot be applied to learn very high dimensional complex embeddings in large knowledge graphs and therefore they have to learn a low

number of very meaningful factors that explain the data. Since all models have to exploit a similar dimensionality for the learned embeddings, the training time and expressiveness of the model will mainly dependent on the optimization algorithm and modeling assumptions. ALS optimized models, i.e. RESCAL, that can exploit closed form solutions allow a faster model optimization than models that exploit stochastic gradient descent. However, as a drawback, the choice of the target loss function is limited to a Gaussian likelihood function. In addition, a closed-world assumption has to be used, which does not consider the notion of missing data. In chapter 5 we will show how local closed-world-assumptions can be exploited to increase RESCAL's capability to consider missing data in its closed form solution updates exploited in ALS (see also [56, 54]). TransE and mwNN are optimized through stochastic gradient descent, which generally lead to longer training times. On the other hand, SGD allows a more careful loss function design which often better represents the underlying assumptions observed in the data regarding missing values and the distribution of the data.

4.2 Simulating Large Scale Conditions

In this section we describe our experimental setup in which we simulate the application of RESCAL, TransE and mwNN to large knowledge graphs. Our experimental setup covers two important aspects:

- We test these models with reasonably low complexity levels, meaning that we enforce low dimensional latent embeddings for entities and relation-types which simulates their application to very large data sets where high dimensional embeddings are intractable. In [25] for example, a latent embedding length (parameter d in Chapter 3.3) of 60 was used.

- We extracted diverse data sets from instances of the Linked-Open Data Cloud, namely Freebase, YAGO and DBpedia, because it is expected that the needed complexity of the models is also dependent on the particular data set the models are applied to. From these knowledge graphs we constructed data sets that will be used as representatives for general purpose knowledge graphs that cover a wide range of relation-types from a diverse set of domains, domain focused knowledge graphs with a specific (smaller) amount of entity classes and relation-types, and high quality knowledge graphs.

Table 4.2: Data sets used in the experiments.

Data Set	Source	Entities	Relation-Types	Triples
DBpedia-Music	DBpedia 2014	321,950	15	981,383
Freebase-150k	Freebase RDF-Dump	151,146	285	1,047,844
YAGOc-195k	YAGO2-Core	195,639	32	1,343,684

In the remainder of this section we will give details on the extracted data sets and the evaluation, implementation and training of RESCAL, TransE and mwNN.

4.2.1 Data Sets

In the following, we describe how we extracted the different data sets from Freebase, DBpedia and YAGO. Note that as described in Chapter 2.1.2, knowledge graphs contain type-constraints that predefine the link structure in graphs; they restrict relation-types to relate only certain classes of entities. We consider these relation-types only in our evaluation, but not in the models, because this is also not done in the original works of these algorithms. Integrating prior knowledge about type-constraints in latent variable models will be covered in Chapter 5. In Table 4.2 some details about the size of these data sets are given.

Freebase-150k

Freebase does not solely rely on structured information extracted from Wikipedia articles, but also integrates information from many other external databases e.g. MusicBrainz, WordNet and many more. Resources in Freebase are referred to as topics. We downloaded the current materialized Freebase rdf-dump[1] and extracted all triples that represent facts involving two Freebase topics that have more than 100 relations to other topics. As a final constraint, we excluded relation-types that are part of less than 100 triples or which did not have both `rdfs:domain` and `rdfs:range` triples. Given the domain and range classes of the relation-types, we also excluded entities that are not an instance of any of those classes. Nevertheless, we observed that some triples violate the extracted type-constraints. Freebase is fairly incomplete and therefore we assumed that these triples are correct, but the inconsistent entities are missing `rdf:type` assignments. We did not try to predict the correct type of the entities in this cases, instead we assumed that these entities belong

[1] https://developers.google.com/freebase/data

to the domain or range of the relation-type where the inconsistency was observed. More technically, if we observe for a triple (s, p, o) that e.g. subject entity s disagrees with the type-constraints of relation-type p, then we simply add the index of entity s to the index vector $\mathbf{domain}_p$, which is used to extract all entities from $\mathcal{E}$ that belong to the domain of relation-type p. This data set will simulate a general purpose knowledge graph in our experiments.

DBpedia-Music

DBpedia contains the structured information extracted from Wikipedia Infoboxes. For the DBpedia-Music data set, we downloaded the owl-ontology, mapping-based-properties (cleaned), mapping-based-types and heuristics from the canonicalized data sets of the current release of DBpedia[2]. We extracted triples from 15 pre-selected Object-Properties; `musicalBand`, `musicalArtist`, `musicBy`, `musicSubgenre`, `derivative`, `stylisticOrigin`, `associatedBand`, `associatedMusicalArtist`, `recordedIn`, `musicFusionGenre`, `musicComposer`, `artist`, `bandMember`, `formerBandMember`, `genre`, where `genre` has been extracted to include only those entities that were covered by the other object-properties to restrict it to musical genres. We discarded all triples of entities that occurred less than twice and for all of the remaining entities that are not assigned to any class, we assigned them to `owl#Thing`. The `rdfs:domain` and `rdfs:range` concepts for the above relation-types were extracted from the DBpedia ontology, where we defined the domain or range of a relation-type as `owl#Thing` if absent. Similar to the Freebase data set, we also observed that some triples disagree with the domain and range constraints of the corresponding relation-type and treated them similarly to the Freebase data set. In our experiments, this data set will simulate a domain specific knowledge graph.

YAGOc-195k

YAGO (Yet Another Great Ontology) is an automatically generated high quality knowledge graph that combines the information richness of Wikipedia Infoboxes and its category system with the clean taxonomy of WordNet. We downloaded the core data set from the YAGO website[3] that contains facts between YAGO-instances. In addition, we downloaded the schema information including the `rdf:type`, `rdfs:range` and `rdfs:domain` triples.[4]

[2] http://wiki.dbpedia.org/Downloads2014

[3] http://www.mpi-inf.mpg.de/departments/databases-and-information-systems/research/yago-naga/yago/downloads/

[4] yagoSchema and yagoTransitiveType

We only included entities that had at least 5 occurrences and that share the types used in the `rdfs:domain` and `rdfs:range` triples. We also excluded relation-types for which less than 100 triples could be observed after pruning the entities could be observed. In contrast to the other two data sets, all triples agreed with the domain and range constraints of the relation-types and therefore no further editing of the data set was needed. This YAGO subsample will be used as representative for a high quality knowledge graph in our experiments.

4.2.2 Evaluation Procedure

We evaluate RESCAL, TransE and mwNN on link prediction tasks, where we delete triples from the data sets and try to re-predict them without considering them during model training. For model training and evaluation we split the triples of the data sets into three sets, where 20% of the triples were taken as holdout set, 10% as validation set for hyper-parameter tuning and the remaining 70% served as training set[5]. In case of the validation and holdout set, we sampled 10 times as many negative triples for evaluation, where the negative triples were drawn such that they did not violate the given domain and range constraints of the knowledge graph. Also, the negative evidence of the holdout and validation set are not overlapping. In knowledge graph data, we are generally dealing with a strongly skewed ratio of observed and unobserved triples, through this sampling we try to mimic this effect to some extent since it is intractable to sample all unobserved triples. After deriving the best hyper-parameter settings for all models, we trained all models with these settings using both the training and the validation set to predict the holdout set (20% of triples). We report the Area Under Precision Recall Curve (AUPRC) for all models. In addition, we provide the Area Under Receiver Operating Characteristic Curve (AUROC), because it is widely used for this problem even though it is not well suited as evaluation measure in these tasks due to the imbalance of (assumed) false and true triples.[6] The discussions and conclusions will be primarily based on the AUPRC results.

We also evaluate the training time of the models, where we measure the runtime in seconds for model training and the number of epochs used until convergence when trained on the validation and training set (80% of triples). In addition we give the mean time per training epoch and the corresponding standard-deviation for better comparison.

[5] Additional 5% of the training set were used for early stopping.

[6] AUROC includes the false-positive rate which relies on the amount of true-negatives that is generally high in these kind of data sets, often leading often to misleading high scores.

4.2.3 Implementation and Model Training Details

All models were implemented in Python using in part Theano [5]. Theano code for TransE is provided by the authors, but we replaced some parts of the original implementation that allowed a significantly faster training.[7] We made sure that our implementation achieved very similar results to the original model on a smaller data set[8] (Results not shown).

The Google Knowledge-Vault multiway neural network (mwNN) was also implemented in Theano. Since there are not many details on model training in the corresponding work [25], we added elastic-net regularization combined with DropConnect [111] on the network weights and optimized the cost function using mini-batch adaptive gradient descent [26]. We randomly initialized the weights by drawing from a zero mean normal distribution where we treat the standard deviation as an additional hyper-parameter. The corrupted triples were sampled with respect to the local closed-world assumption discussed in [25]. We fixed the amount of corrupted triples per training example to five.[9]

For RESCAL, we used the ALS implementation provided by the author[10], but extended it in such a way that it supports a more scalable early stopping criteria based on a small validation set.

For hyper-parameter tuning, all models were trained for a maximum of 50 epochs and for the final evaluation on the holdout set for a maximum of 200 epochs. For all models, we sampled 5% of the training data as validation set and computed the change in AUPRC for early stopping on this set. For ALS, we stopped training if the AUPRC score did not increase more than $1E^{-4}$ for five epochs in a row and kept the best known configuration. In case of the SGD optimized models, we computed the AUPRC twice in an epoch and stopped training after the AUPRC score has also not increased 10 times in a row for $1E^{-4}$.

All models were trained with an Intel Xeon E5-2680 v2 (Amazon EC2 c3 instance) using 4 threads (OpenBLAS).

[7] Slower runtime is mainly caused by the ranking function used for calculating the validation error, but the consideration of trivial zero gradients during the SGD-updates also caused slowdowns.

[8] http://alchemy.cs.washington.edu/data/cora/

[9] We tried different amounts of corrupted triples and five gave the most stable results across all data sets.

[10] https://github.com/mnick/scikit-tensor

Table 4.3: AUPRC and AUROC results of RESCAL, TransE and mwNN on the Freebase-150k data set. The right columns show total training time, epochs needed for training, mean time per epoch, standard deviation of training times per epoch.

		Freebase-150k					
Model	**d**	**AUPRC**	**AUROC**	**Train(s)**	**Epochs**	μ_{Time}	σ_{Time}
RESCAL	10	0.327	0.616	**101**	**6**	**12.2**	2.5
TransE	10	**0.548**	**0.886**	11,942	148	80.5	1.2
mwNN	10	0.437	0.852	1,730	18	92.0	7.8
RESCAL	50	0.453	0.700	**371**	**6**	**49.2**	7.8
TransE	50	**0.715**	**0.890**	18,020	120	149.5	5.1
mwNN	50	0.471	0.868	2,115	14	144.2	12.1
RESCAL	100	0.514	0.753	**1,723**	**13**	**118.8**	11.7
TransE	100	**0.743**	**0.892**	18,515	73	252.1	1.1
mwNN	100	0.512	0.879	5,568	21	254.1	18.4

4.3 Experimental Results

Below, we provide the empirical results for RESCAL, TransE and mwNN with respect to their link prediction quality and training times at different levels of model complexity (varying the dimensionality d of the latent embeddings) on the data sets described in Section 4.2.1. The results can be seen in Table 4.3,4.4 and 4.5. These tables follow the same structure, where each table represents our measurements for all three models with respect to one data set, e.g. Table 4.3 shows the link-prediction results and training time measurements for RESCAL, TransE and mwNN for the Freebase-150k data set. The first four columns show the AUPRC and AUROC scores achieved in the link-prediction task by each model with respect to the chosen embeddings dimension **d**. The last four columns describe the corresponding training time measurements for these models: Total training time in seconds, epochs needed until convergence, mean time per epoch in seconds [11].

4.3.1 Link-Prediction Quality – TransE has Leading Performance

From the AUPRC results shown in Table 4.3,4.4 and 4.5, it can be clearly concluded that TransE achieves the highest link-prediction quality on all data sets and all allowed latent embeddings vector lengths. Even at the lowest model complexity with an embedding length of 10, it outperforms the other models even if these models exploit higher dimensional

[11] These are the pure times per epoch excluding other pre-computations like e.g. initialization etc., and as a consequence $\mu_{\text{Time}} * Epoch \leq Train(s)$.

Table 4.4: AUPRC and AUROC results of RESCAL, TransE and mwNN on the DBpedia-Music data set. The right columns show total training time, epochs needed for training, mean time per epoch, standard deviation of training times per epoch.

DBpedia-Music							
Model	**d**	**AUPRC**	**AUROC**	**Train(s)**	**Epochs**	μ_{Time}	σ_{Time}
RESCAL	10	0.307	0.583	**40**	**6**	**4.8**	0.5
TransE	10	**0.701**	**0.902**	7,496	108	69.3	2.3
mwNN	10	0.436	0.836	564	10	53.9	0.4
RESCAL	50	0.362	0.617	**205**	**11**	**15.7**	4.1
TransE	50	**0.748**	**0.911**	13,316	72	182.3	9.2
mwNN	50	0.509	0.864	5,043	25	198.0	19.8
RESCAL	100	0.416	0.653	**503**	**13**	**33.1**	8.8
TransE	100	**0.745**	**0.903**	62,072	76	811.9	21.1
mwNN	100	0.538	0.865	8,950	31	282.6	19.2

embeddings. For example, on the Freebase-150k data set TransE achieves an AUPRC score of 0.548 ($\mathbf{d} = 10$), where RESCAL and mwNN achieve only 0.514 and 0.512, respectively, with an embedding length of 100. On the DBpedia-Music and YAGOc-195k we can observe similar differences in AUPRC.

RESCAL seems to have problems in capturing structure of the data when exploiting very low dimensional embeddings ($\mathbf{d} = 10$). On all data sets, it clearly has the lowest link-prediction quality in these cases, achieving only an AUPRC of 0.327 (Freebase-150k), 0.307 (DBpedia-Music) and 0.507 (YAGOc-195k). In the first two cases, the best configuration is already found after one epoch (Epoch=6 in the Tables 4.3 and 4.4 [12]). In order to rule out any issues with the early stopping criteria, we let RESCAL train for more epochs in a separate experiment, but the AUPRC score was indeed getting worse, because the latent factors were pushed against zero.

The neural network model performs better than RESCAL with very low-dimensional embeddings, achieving an AUPRC score of 0.437 (Freebase-150k) , 0.436 (DBpedia-Music), and 0.600 (YAGOc-195k), where RESCAL only achieved 0.327, 0.307 and 0.507. We assume that the non-linear interaction of the embeddings in the neural network layers help the model to capture data structure at this low model complexity level. With longer embeddings of $\mathbf{d} = 100$, RESCAL catches up to mwNN and even outperforms it in some cases. On the general purpose knowledge graph (Freebase-150k), both have similar link-prediction quality (Table 4.3), where mwNN outperforms RESCAL in case of the domain

[12]Training is stopped if the AUPRC is not improved after 5 epochs, we keep the best configuration.

Table 4.5: AUPRC and AUROC results of RESCAL, TransE and mwNN on the YAGOc-195k data set. The right columns show total training time, epochs needed for training, mean time per epoch, standard deviation of training times per epoch.

YAGOc-195k							
Model	**d**	**AUPRC**	**AUROC**	**Train(s)**	**Epochs**	μ_{Time}	σ_{Time}
RESCAL	10	0.507	0.621	**117**	**21**	**5.0**	0.4
TransE	10	**0.793**	0.904	9,862	113	86.6	1.3
mwNN	10	0.600	**0.949**	4,508	45	99.5	6.1
RESCAL	50	0.694	0.787	**210**	**13**	**13.9**	2.1
TransE	50	**0.849**	**0.960**	7,928	41	190.5	10.1
mwNN	50	0.684	0.949	5,742	23	241.5	21.3
RESCAL	100	0.721	0.800	**576**	**18**	**28.3**	4.4
TransE	100	**0.816**	0.910	15,682	43	360.0	13.4
mwNN	100	0.655	**0.957**	10,434	36	288.7	16.8

specific DBpedia-Music data set (Table 4.4) and RESCAL outperforms mwNN in case of the high quality YAGOc-195k data sets (Table 4.5).

4.3.2 Optimization Time – RESCAL is Superior to Other Methods

In this subsection we have a closer look at some practical aspects observed when training the different models. In the right columns of the tables 4.3,4.4 and 4.5, we give some characteristic measurements regarding the training of the different models. As expected, RESCAL has generally the lowest total training times and mean time per epoch, especially with latent embedding vectors of length 10. In addition, RESCAL has only two additional hyper-parameters that control the L_2-regularization of the factor matrix $\mathbf{A}$ and core tensor $\underline{\mathbf{R}}$. The combination of simplicity and speed makes RESCAL especially suitable for quick solutions in large scale problems.

TransE on the other hand clearly has the longest training times, even though it is quite simple. For the Freebase data set and all different embedding dimensions, it took between 3-5h (11,942-18,515 sec) to train this model until convergence, whereas the neural network took only 0.5-1.5h (1,730 - 5,568 sec) and RESCAL ran 2 minutes to half an hour. The main reason for this lies in the fact that it needs the most epochs until convergence due to its fixed learning rates. It is worth noticing that the training time per epoch is increasing dramatically on the DBpedia-Music data set when an embedding length of 100 is used.

The DBpedia-Music data set has the most entities (321,950) and TransE seems to be more sensitive to an increase in the size of entities. We profiled the code to ensure that this increase in time was not caused by some inefficient code snippet and observed that the main part of the runtime is indeed spent in the gradient calculation. Furthermore, we found this model quite straight-forward to tune (only three additional hyper-parameters), but its long training times limit its applicability to very large data sets. Note that our implementation of this models is already magnitudes faster than the original code provided by the authors, which took over a day to converge on these data sets.

In exception to the previously mentioned case where TransE's training time per epoch dramatically increased on the DBpedia-Music data set, the mwNN model has similar training times per epoch as TransE. However, the total training time of mwNN is significantly lower since it needs significantly less epochs to convergence due to the adaptive gradient optimization. As a drawback, we found this model quite hard to tune, because it has a multitude of hyper-parameters. We clearly spent the most effort here.

4.4 Related Work

Tensors have been applied to Web analysis in [52] and for ranking predictions in the Semantic Web in [35]. [90] applied tensor models to rating predictions. Using factorization approaches to predict ground atoms was pioneered in [104]; [82], [113], [11], and [50] applied tensor models for this task, where [82] introduced the RESCAL model. [94] applied matrix factorization for relation extraction in universal schemas. The RESCAL model has been the basis of multiple recently published works: [55] introduced non-negative constraints, [81] presented a logistic factorization and [50] explicitly models the 2nd and 3rd order interactions.

[99] recently proposed a neural tensor network which we did not consider in our study since it was observed that it does not scale to larger data sets [17, 25]. Instead we exploit a less complex and more scalable neural network model proposed in [25] which could achieve comparable results to the neural tensor network of [99].

[12] proposed the Semantic Matching Energy model (SME), which was later refined and improved in scalability by the translational embeddings model (TransE) introduced in [9]. Entities and relation-types are represented by latent embedding vectors in these models and the score of a triple is measured in terms of a distance-based similarity measure as motivated by [74, 73]. TransE [9] has been he target of other recent research activities. [114]

proposed a framework for relationship modeling that combines aspects of TransE and the neural tensor network proposed in [99]. [112] proposed TransH which improves TransE's capability to model reflexive one-to-many, many-to-one and many-to-many relation-types by introducing a relation-type-specific hyperplane where the translation is performed. This work has been further extended in [67] by introducing TransR which separates representations of entities and relation-types in different spaces, where the translation is performed in the relation-space. An extensive review on representation learning with knowledge graphs can be found in [80].

Latent variable methods have been combined with graph-feature models which lead to an increase of prediction quality [25] and a decrease of model complexity [79]. Further, it has been shown in [54] that the prediction quality of latent variable models, such as RESCAL, TransE and the neural network used in the Google Knowledge Vault system, can also be significantly improved at lower model complexities by integrating prior knowledge on relation-types, i.e. type-constraints extracted from the knowledge graph schema.

General methods for link-prediction also include Markov-Logic-Networks [92] which have a limited scalability and random walk algorithms like the path ranking algorithm [60].

4.5 Conclusion

For the statistical modeling of large knowledge graphs, latent variable models require to capture the dependencies in the graph within low dimensional latent embeddings of entities and relation-types, since high dimensional embeddings can cause intractable training times and memory loads. As an example, the embeddings matrix for the whole of Freebase (~ 40 million entities, i.e. topics) will consume 16 TB of memory if an embedding length of 100,000 would be chosen (considering single precision floats). The computational costs of such huge embedding matrices will be tremendous.

From the experimental results discussed in Section 4.3.1, we can conclude that TransE is most capable of learning meaningful low dimensional embeddings, but with the price of significantly higher training times than RESCAL. RESCAL on the other hand has a significantly worse link-prediction quality than TransE when exploiting very low dimensional embeddings, but is optimized extremely fast. Opposing these two extremes, one difference becomes directly apparent: the way these models handle missing data. TransE optimizes a max-margin ranking loss function that considers every triple as missing that is not observed in the data. Therefore, the loss function focuses on highlighting the true

triples in the data. RESCAL on the other hand uses a closed-world assumption. RESCAL factorizes a large third order tensor and optimizes a reconstruction penalty that considers all possible combinations of triples in the data in every update. It is not surprising that, due to the overwhelming amount of assumed negative evidence in the data, the reconstruction error is best minimized by approximating a tensor with almost no signals (everything is zero) if a low amount of parameters is available. The mwNN model is in the middle of the other two models in terms of prediction quality when exploiting very low dimensional embeddings, probably due to its local closed-world assumption that includes aspects of both approaches. In the case of RESCAL or mwNN there have been extensions proposed that combine them with graph feature models to increase their link-prediction capabilities with lower dimensional embeddings [79, 25].

However, even though the aspect of missing data seems a plausible explanation for the observed differences in quality of the prediction results between all three models, it masks one important aspect of knowledge graphs that is not considered by any of these methods, –a knowledge graph is not a complete graph–. In addition to true, missing and (assumed) false triples we have to deal with the fact that there are combinations of entities and relation-types that should not occur at all, because they do not make any sense. The differentiation from these "impossible" triples is provided through type-constraints on relation-types (see Chapter 2.1.2). Incorporating this kind of prior knowledge on the graph structure dramatically decreases the amount of possible worlds the latent variable models have to consider when modeling knowledge graphs. In the next chapter we will show how this prior knowledge can be integrated in latent variable models and study their general value for the statistical modeling of knowledge graphs with latent variable models.

Chapter 5

Exploiting Prior Knowledge On Relation-Type Semantics

We have illustrated in Chapter 2.1.2 that besides storing facts about the world, schema-based knowledge graphs are backed by rich semantic descriptions of entities and relation-types that allow machines to understand the notion of things and their semantic relationships. Generally, entities in knowledge graphs like DBpedia, Freebase or YAGO are assigned to one or multiple predefined classes (or types) that are organized in an often hierarchical ontology. These assignments represent for example the knowledge that the entity `Albert Einstein` is a person and therefore allow a semantic description of the entities contained in the knowledge graph. The organization of entities in semantically meaningful classes further permits a semantic definition of relation-types. The RDF-Schema offers among others the concepts `rdfs:domain` and `rdfs:range` for this purpose. Annotations that describe relation-type semantics provide valuable information to machines, e.g. that the `marriedTo` relation-type should relate only instances of the class `person`.

In this chapter we study the general value of prior knowledge about the semantics of relation-types and entities for the statistical modeling of knowledge graphs with latent variable models. We show how the annotated semantics provided by the `rdfs:domain` and `rdfs:range` concepts can be effectively exploited in latent variable models, thereby improving the link prediction quality significantly on various data sets.

Additionally, we address the issue that type-constraints can also suffer from incompleteness; `rdfs:domain` or `rdfs:range` concepts are absent in the schema or the entities miss proper typing even after materialization. In this regard, we motivate and study a local closed-world assumption that approximates the semantics of relation-types solely based

on observed triples in the graph. We provide empirical proof that this prior assumption on relation-types generally improves link-prediction quality in case proper type-constraints are absent or fuzzy.

This chapter is structured as follows: In the following section, we extend RESCAL's efficient optimization algorithm such that type-constraints are considered without loosing the its great scalability properties. Furthermore, we discuss a series of proof of concept experiments which show that RESCAL benefits to a large extent from the integration of prior knowledge on relation-types. The integration of prior knowledge about type-constraints is not limited to RESCAL, but can also be integrated in the stochastic gradient optimized models exploited by TransE and mwNN. We show how this can be accomplished in in Section 5.2. In Section 5.3 we motivate and describe a local closed-world assumption on relation-types that can be exploited by latent variable models in case proper type-constraints are absent or fuzzy. In the final part of this chapter (Section 5.4) , we analyze the general value of type-constraints and the proposed local closed-world assumption in more detail based on extensive experiments on all models and various representative data sets. We provide related work in Section 5.5 and conclude in Section 5.6.

Own contributions in this chapter are published in

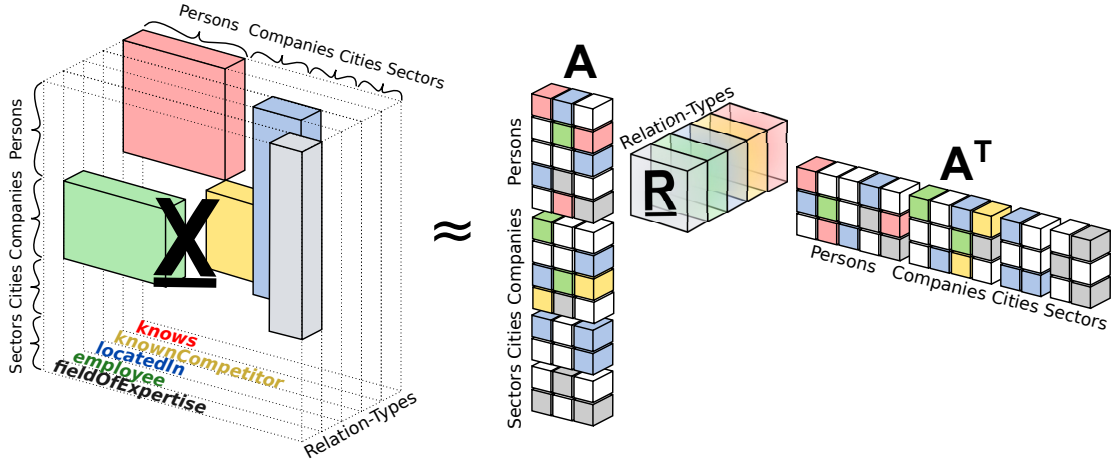
[56] Denis Krompaß, Maximilian Nickel and Volker Tresp. *Large-Scale Factorization of Type-Constrained Multi-Relational Data.* International Conference on Data Science and Advanced Analytics (DSAA2014), 2014.

[54] Denis Krompaß, Stephan Baier and Voker Tresp. *Type-Constrained Representation Learning in Knowledge-Graphs.* In Proceedings of the 14th International Semantic Web Conference (ISWC), 2015

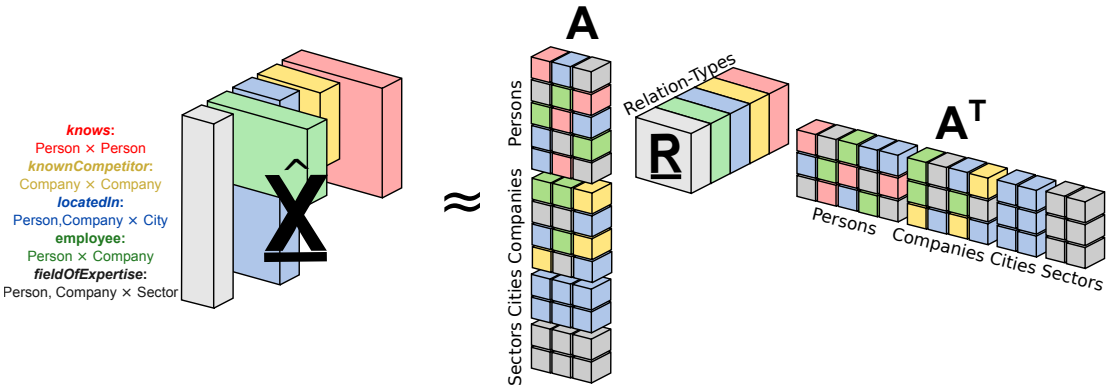
where Section 5.1 and Section 5.3 cover the main contributions published in [56] but with improved notation. The contributions published in [54] are depicted in Section 5.2 and Section 5.4.

5.1 Type-Constrained Alternating Least-Squares for RESCAL

RESCAL as proposed by [82][83] does not consider or support type-constraints, but posts a closed-word assumption on the complete adjacency tensor. A closed-world assumption



(a) A partially observed tensor that is factorized by RESCAL



(b) Factorizing with respect to domain and range constraints of the relations

Figure 5.1: Schematic of factorizing knowledge-graph data with RESCAL without (a) and with (b) considering type-constraints. For better understanding, we used data from a hypothetical knowledge-graph in the figures. The colored boxes on the left side of the equations represent the regions in the adjacency matrices that are defined by the domain and range constraints. Every entry in the adjacency tensor that is not within these colored regions violates these constraints. In both approaches (a,b), the data is factorized into the same latent factor structure, a shared latent representation for the entities (factor matrix $\mathbf{A}$) and an interaction core tensor $\underline{\mathbf{R}}$. By the coloring of the right factor matrices we illustrate which data from the left side has impact on the latent representations. The difference between considering and not considering the given type-constraints becomes clear when comparing for example the latent representations of cities. Only the triples that relate cities and that lie in the blue region in the tensor are actually defined, but the original RESCAL additionally includes unobserved relations of cities (as negative evidence) that lie outside of this region due to its closed-world assumption. By integrating type-constraints into the model, only triples from the colored regions are exploited in the factorization (b).

corresponds to the assumption that an entity can be related to any other known entity in the database. Especially in general purpose knowledge graphs such as Freebase or DBpedia this assumption has many disadvantages. Most of the relation-types are specialized to express relations between certain classes of entities, explicitly excluding a vast amount of relations to other entity classes. In Figure 5.1.a we illustrate this by an example regarding a hypothetical knowledge-graph about companies and their employees. For RESCAL, the data is stored in a three-way adjacency tensor (Chapter 3.3.2), but in difference to multi-relational data sets e.g. the Nations or Kinship data sets[1], the different relation-types are not always defined for all the entities. Instead, we are dealing with a partially observed tensor where, as indicated by the colored blocks in the adjacency tensor, the potentially observable parts are predefined through each relation-type's type-constraints[2]. For example, the relation-type `knownCompetitor` only relates entities of the class `company` to each other (red block in last frontal slice) or the relation-typ `employee` relates entities of the class `company` with entities of the class `person` (green block in second frontal slice of tensor $\underline{\mathbf{X}}$ in Figure 5.1.a). On the other hand, obviously meaningless relations between the same class of entities (persons and companies) using the `fieldOfExpertise` relation-type are excluded (e.g. the relation (`John_Smith`, `fieldOfExpertise`, `IBM`)).

By ignoring prior knowledge about type-constraints all possible combinations of entities and relation-types are considered during factorization that include a vast amount of meaningless triples. These meaningless triples have a significant impact on the embeddings of entities and relation-types learned by RESCAL. In addition, they increase the sparsity of the adjacency tensor by several magnitudes, what causes additional problems by its own when factorizing the data. It is expected that the larger and heterogeneous the knowledge graph, the more of these trivial false triples are implicitly represented in the tensor and the more severe is the impact on the factorization and the latent embeddings.

To understand the problem in more detail, we have to take a closer look at how RESCAL learns the embeddings during factorization. Let us consider the relation-type `locatedIn` in Figure 5.1.a. The blue block in the adjacency tensor represents the triples that agree with the type-constraints, namely entities of the classes `person` and `company` are being related to instances of the class `city`. By considering the RESCAL update for the latent

[1] http://alchemy.cs.washington.edu/data/

[2] Assuming a clean knowledge graph as for example YAGO where all relation-types have such constraints.

embedding of entities

$$A = [\sum_k \mathbf{X}_k \mathbf{A}\mathbf{R}_k^T + \mathbf{X}_k^T \mathbf{A}\mathbf{R}_k][\sum_k \mathbf{R}_k \mathbf{A}^T \mathbf{A}\mathbf{R}_k^T + \mathbf{R}_k^T \mathbf{A}^T \mathbf{A}\mathbf{R}_k]^{-1},$$

and especially the part that covers relation-type `locatedIn`

$$\begin{aligned} A \;=\; & [... + \mathbf{X}_{locatedIn} \mathbf{A}\mathbf{R}_{locatedIn}^T + \mathbf{X}_{locatedIn}^T \mathbf{A}\mathbf{R}_{locatedIn} + ...] \\ & [... + \mathbf{R}_{locatedIn} \mathbf{A}^T \mathbf{A}\mathbf{R}_{locatedIn}^T + \mathbf{R}_{locatedIn}^T \mathbf{A}^T \mathbf{A}\mathbf{R}_{locatedIn} + ...]^{-1} \end{aligned} \tag{5.1}$$

where $\mathbf{X}_{locatedIn}$ is the adjacency matrix for the relation-type `locatedIn`, $\mathbf{A}$ and $\mathbf{R}_{locatedIn}$ are the embedding matrices for the entities and the relation-type, respectively, it can be directly seen that RESCAL does not consider prior knowledge about type-constraints. The top part of Equation 5.1 that contains the sparse adjacency matrix $\mathbf{X}_{locatedIn}$ causes not any problems, since all unobserved entities are multiplied by zero and drop out of the equation. However, in the lower part of the Equation 5.1 (the inverse), the embedding of every entity is considered for all relation-types, thereby having a tremendous impact on the inverse and the final update of the entity embeddings. This observation is illustrated by the different coloring in factor matrix $\mathbf{A}$ in Figure 5.1.a. Besides the triples (observed and unobserved) that agree with the type-constraints, also triples that violate them contribute to the learned latent embeddings (indicated by the white boxes).

Accordingly, since the latent embedding matrices of relation-types are dependent on the complete set of latent embeddings of the entities during model training[3], they are considering explicitly all possible relations between entities and therefore a vast amount of meaningless triples. We highlight this fact by the blur or the core-tensor $\underline{\mathbf{R}}$ in Figure 5.1.a.

For larger knowledge graphs, the overwhelming number of negative evidence (meaningless triples are treated as negative evidence due to the closed-world assumption) will push the factors to zero because of the reconstruction penalty (Equation 3.1), especially when pursuing a low rank factorization (which we are interested in). Of course, this can be counteracted by choosing a sufficiently high rank that allows the model to spend some parameters to learn the rarely observed true signals in the data. This approach can suffice for small data sets but as discussed in Chapter 4, with real knowledge graphs that contain millions of entities a high rank factorization can quickly become intractable; A high rank

[3]The R-update of RESCAL relies on the Singular-Value-Decomposition of the factor matrix $\mathbf{A}$.

has a dramatic impact on the runtime[4] and memory consumption of RESCAL.

In order to integrate type-constraints as given by the `rdfs:domain` and `rdfs:range` triples, we have to guarantee that all triples that violate the type-constraints are ignored for all relation-types during factorization. In other words, for each relation-type we want to factorize the corresponding knowledge-graph with respect to the subset of entities that agrees with the type-constraints and suits the semantics of the corresponding relation. Therefore, the factorization of each frontal slice of the adjacency tensor, in which each frontal slice represents an adjacency matrix for one relation-type, might be completely different in shape to the ones of the other frontal slices (Figure 5.1.b) because we exclude entities. Strictly speaking, we dismiss the representation of the triples in a uniformly shaped third-order adjacency tensor in favor of a list of frontal slices of arbitrary shape in which each of these frontal slices explicitly excludes triples that violate the corresponding type-constraints. Nevertheless, we want to exploit the same factorization structure than RESCAL, but where each adjacency matrix of the relation-types only influences the latent embeddings of a smaller subset of entities unless all entities are included in the union of classes covered by the domain and range constraints. The goal of this approach is indicated by the factorization in Figure 5.1.b, the latent embeddings are clean. By "clean" we mean that no meaningless triples contribute to the latent embeddings of entities or relation-types (no white boxes in $\mathbf{A}$ and no blur in core tensor $\underline{\mathbf{R}}$).

Factorizing the list of frontal slices efficiently can be achieved by integrating the type-constraints directly into the RESCAL Least-Squares cost function and by exploiting a similar Alternating Least-Squares optimization scheme. For this reason, the type-constraints have to be encoded in a way that can be exploited by the optimization algorithm as we will show next.

5.1.1 Additional Notation

In addition to the notation used in Chapter 3.3.1, $\hat{\mathbf{X}}_k$ will denote the frontal-slice $\mathbf{X}_k$ where only subject entities (rows) and object entities (columns) are included that agree with the domain and range constraints of relation-type k. Additionally, we denote $\mathbf{X}_{[\mathbf{z},:]}$ for the indexing of multiple rows from the matrix $\mathbf{X}$, where $\mathbf{z}$ is a vector of indices and ":" the colon operator generally used when indexing arrays. We further denote $\mathbf{domain}_k$ as the sorted indices of all entities that agree with the domain constraints of relation-type k. Accordingly, $\mathbf{range}_k$ denotes these indices for the range constraints of relation-type k.

[4]RESCAL scales cubic with the rank.

5.1.2 Integrating Type-Constraints into RESCAL

The integration of type-constraints in the RESCAL ALS optimization algorithm requires a suitable representation of these type-constraints. We represent the type-constraints for each relation-type as two vectors containing unique entity indices that we construct a priori from the data and the given `rdfs:domain` and `rdfs:range` concepts. These entity indices correspond to the order of entities in the latent entity embedding matrix $\mathbf{A}$ (and the tensor $\underline{\mathbf{X}}$). We denote these vectors as $\mathbf{domain}_k$ and $\mathbf{range}_k$, where the former contains the indices of entities that belong to classes defined by the domain and the latter to the classes defined by the range of the relation-type k. These index vectors are exploited to extract the sub-adjacency matrices from each frontal slice in the adjacency tensor $\underline{\mathbf{X}}$ to construct the previously mentioned new representation of the knowledge graph as a list of adjacency matrices of arbitrary shape (Figure 5.1.b). By exploiting this new data representation and the two index vectors, RESCAL's regularized Least-Squares cost function is adapted to

$$\mathcal{L} = \sum_k \|\hat{\mathbf{X}}_k - \mathbf{A}_{[\mathbf{domain}_k,:]}\mathbf{R}_k\mathbf{A}^T_{[\mathbf{range}_k,:]}\|_F^2 + \lambda_A\|\mathbf{A}\|_F^2 + \lambda_R\sum_k \|\mathbf{R}_k\|_F^2, \tag{5.2}$$

where $\mathbf{A}$ represents the latent embeddings for the entities and $\mathbf{R}_k$ the embeddings for the relation-type k. For each relation-type k the latent embedding matrix $\mathbf{A}$ is indexed by the corresponding domain and range constraints in order to exclude all entities that disagree with the type constraints. $\hat{\mathbf{X}}_k$ denotes the adjacency matrix for the subgraph that agrees with the type-constraints of relation-type k. Note that, if the adjacency matrix $\hat{\mathbf{X}}_k$ defined by the sub-graph of relation-type k and its type-constraints has the shape $n_k \times m_k$, then $\mathbf{A}_{[\mathbf{domain}_k,:]}$ is of shape $n_k \times d$ and $\mathbf{A}_{[\mathbf{range_k},:]}$ is of shape $m_k \times d$, where d is the dimension of the latent embeddings (or rank of the factorization).

Even though the cost function defined in Equation 5.2 looks very similar to the cost function of RESCAL (Equation 3.1), it contains important differences since we are actually factorizing a list of matrices of arbitrary shapes (denoted by the "ˆ") instead of uniformly shaped frontal tensor slices. However, through the similar formulation of the optimization problem we are still able to exploit the nice scalability properties of RESCAL. In the next two subsections, we provide details on the ALS updates of the factor matrix $\mathbf{A}$ and the core Tensor $\underline{\mathbf{R}}$ of type-constrained RESCAL. The full algorithm is illustrated in Algorithm 1, where $\mathbf{domain}_{\underline{\mathbf{X}}}$ denotes the list of index vectors $\mathbf{domain}_k$ and $\mathbf{range}_k$ for each relation-type k present in the data (tensor $\underline{\mathbf{X}}$).

Algorithm 1 Type-Constrained RESCAL

Require: Adjacency Tensor: $\underline{\mathbf{X}}$, Type-Constraints in $\underline{\mathbf{X}}$: ($\mathbf{domain}_{\underline{\mathbf{X}}}$,$\mathbf{range}_{\underline{\mathbf{X}}}$)

function RESCAL_TC($\underline{\mathbf{X}}, r, \lambda_A, \lambda_R, \mathbf{domain}_{\underline{\mathbf{X}}}, \mathbf{range}_{\underline{\mathbf{X}}}$) ▷ r: rank of factorization, λ_A, λ_R: regularization parameters
  $\hat{\underline{\mathbf{X}}} = shrinkX(\underline{\mathbf{X}}, \mathbf{domain}_{\underline{\mathbf{X}}}, \mathbf{range}_{\underline{\mathbf{X}}})$ ▷ Apply Type-Constraints on $\underline{\mathbf{X}}$
  $\mathbf{A}$,$\underline{\mathbf{R}} = initialize(\underline{\mathbf{X}},r)$ ▷ based on eigendecomposition of $\sum_k(\mathbf{X}_k + \mathbf{X}_k^T)$ [3]
  repeat
    $\mathbf{A} \leftarrow updateA(\hat{\underline{\mathbf{X}}}, \mathbf{A}, \underline{\mathbf{R}}, \mathbf{domain}_{\underline{\mathbf{X}}}, \mathbf{range}_{\underline{\mathbf{X}}}, \lambda_A)$ ▷ Equation 5.3
    $\underline{\mathbf{R}} \leftarrow updateR(\hat{\underline{\mathbf{X}}}, \mathbf{A}, \mathbf{domain}_{\underline{\mathbf{X}}}, \mathbf{range}_{\underline{\mathbf{X}}}, \lambda_R)$ ▷ Equation 5.5
  until convergence or max iteration reached
  return $\mathbf{A}$,$\underline{\mathbf{R}}$
end function

Type-Constrained Update of the Factor Matrix A

For the ALS updates, we exploit the indexing on factor matrix $\mathbf{A}$ to avoid the impact of type-constraint violating triples on the latent embeddings. However, due to the introduced variety caused by the different type-constraint definitions for each relation-type k, some computational overhead compared to the original updates has to be introduced. For the latent embedding of the i-th entity we get

$$\begin{aligned} \mathbf{a}_i \quad &= \quad \left[\sum_k \hat{\mathbf{X}}_k \mathbf{A}_{[\mathbf{range}_k,:]} \mathbf{R}_k^T + \hat{\mathbf{X}}_k^T \mathbf{A}_{[\mathbf{domain}_k,:]} \mathbf{R}_k\right]_i \left[\sum_k \mathbb{1}_{\mathbf{domain}_k}(i)\mathbf{E}_k + \mathbb{1}_{\mathbf{range}_k}(i)\mathbf{F}_k\right]^{-1} \\ with \quad & \mathbf{E}_k = \mathbf{R}_k \mathbf{A}_{[\mathbf{range}_k,:]}^T \mathbf{A}_{[\mathbf{range}_k,:]} \mathbf{R}_k^T, \; \mathbf{F}_k = \mathbf{R}_k^T \mathbf{A}_{[\mathbf{domain}_k,:]}^T \mathbf{A}_{[\mathbf{domain}_k,:]} \mathbf{R}_k \end{aligned} \tag{5.3}$$

where $\mathbf{a}_i$ is the i-th row vector of A that represents the latent embedding of the i-th entity and $\mathbb{1}$ is the indicator function. $\mathbb{1}_{\mathbf{domain}_k}$ denotes the indicator function of the set of entity indices contained in the domain of relation-type k and $\mathbb{1}_{\mathbf{range}_k}$ vice versa for the range. The most obvious difference to the original RESCAL $\mathbf{A}$-update lies in the fact that we cannot update the complete factor matrix $\mathbf{A}$ as efficiently at once. The original update only requires the calculation of one inverse that can be exploited for all latent embeddings of entities. In the new update, the inverse in Equation 5.3 is dependent on the range and domain constraints and whether the entity is included or excluded by those constraints for each relation-type k as subject or as object. Each indicator function $\mathbb{1}$ sets one whole summand to zero if the index of an entity is not included in the index vector for the

domain or the range, respectively. Note that in the current form, we have to calculate as many inverses as there are entities in the knowledge graph. This can become extremely expensive when a high rank for the factorization is used (the inverse of $d \times d$ matrices have to be computed). Fortunately, we can exploit the fact that domain and range constraints are on class level and therefore entities of the same class are sharing the same inverses, reducing the number of computed inverses per update in the worst to the number of classes covered by the type-constraints. In addition, we discussed Chapter 4 that d is required to be small when RESCAL is applied to large knowledge graphs leading to significantly reduced computational loads when computing the inverses.

On the other hand, some computation have become more efficient because they incorporate on the much smaller matrices $\hat{\mathbf{X}}_k^T$, $\mathbf{A}_{[\mathbf{domain}_k,:]}$ and $\mathbf{A}_{[\mathbf{range}_k,:]}$ for each relation-type.

Type-Constrained Update of Core Tensor $\underline{\mathbf{R}}$

We are still able to utilize an efficient closed-form solution for the update of the latent embeddings for relation-types (core tensor $\underline{\mathbf{R}}$). Nevertheless, we have to consider that each frontal slice $\mathbf{R}_k$ has to be updated with respect to two different sets of latent embedding vectors contained in $\mathbf{A}$, namely $\mathbf{A}_{[\mathbf{domain}_k,:]}$ and $\mathbf{A}_{[\mathbf{range}_k,:]}$. For each frontal slice of $\underline{\mathbf{R}}$ we get the following closed-form solution for the update:

$$\begin{aligned} \mathbf{R}_k \quad &= \quad ((\mathbf{C} \otimes \mathbf{B})^T(\mathbf{C} \otimes \mathbf{B}) + \lambda \mathbf{I})^{-1}(\mathbf{C} \otimes \mathbf{B})^T vec(\hat{\mathbf{X}}_k) \\ &with \quad \mathbf{B} = \mathbf{A}_{[\mathbf{domain}_k,:]} \; and \; \mathbf{C} = \mathbf{A}_{[\mathbf{range}_k,:]}. \end{aligned} \tag{5.4}$$

As in [78], we can exploit the following property of the singular value decomposition (SVD) regarding the Kronecker product of two matrices [62]

$$\mathbf{C} \otimes \mathbf{B} = (\mathbf{U_C} \otimes \mathbf{U}_B)(\Sigma_\mathbf{C} \otimes \Sigma_\mathbf{B})(\mathbf{V_C}^T \otimes \mathbf{V}_B^T),$$

with $\mathbf{B} = \mathbf{U_B}\mathbf{\Sigma_B}\mathbf{V_B}^T$ and $\mathbf{C} = \mathbf{U_C}\mathbf{\Sigma_C}\mathbf{V_C}^T$, leading to the much more efficient update for $\mathbf{R}_k$

$$\mathbf{R}_k = \mathbf{V_B}(\mathbf{P} \circledast \mathbf{U_B}^T\hat{\mathbf{X}}_k\mathbf{U_C})\mathbf{V_C}^T \tag{5.5}$$

where $\circledast$ denotes the Hadamard product and $\mathbf{P}$ is defined as follows: Let $\mathbf{Q}$ be defined as a diagonal matrix and where its diagonal entry q_{ii} is given by

$$\begin{aligned} q_{ii} &= \frac{\mathbf{D}_{\mathbf{B}_{ii}}\mathbf{D}_{\mathbf{C}_{ii}}}{\mathbf{D}^2_{\mathbf{B}_{ii}}\mathbf{D}^2_{\mathbf{C}_{ii}} + \lambda} \\ \text{with } \mathbf{D}_{\mathbf{B}} &= \Sigma_{\mathbf{B}} \otimes \Sigma_{\mathbf{B}} \text{ and } \mathbf{D}_{\mathbf{C}} = \Sigma_{\mathbf{C}} \otimes \Sigma_{\mathbf{C}}. \end{aligned}$$

Then $\mathbf{P}$ can be constructed by a column-wise reshape of the diagonal in $\mathbf{Q}$.

Note, that we are generally dealing with different domain and range constraints for each relation, therefore $\mathbf{A}_{[\mathbf{domain}_k,:]}$ and $\mathbf{A}_{[\mathbf{range}_k,:]}$ will differ for each R_k. In contrast to the updates in RESCAL we cannot use the result of one *SVD* on the factor matrix $\mathbf{A}$ for all frontal slice updates of $\underline{\mathbf{R}}$. In our case we have to perform two *SVD*s for each updated $\mathbf{R}_k$. This seems less efficient at the first moment, but the *SVD*s are only calculated on the much smaller factor matrices $\mathbf{A}_{[\mathbf{domain}_k,:]}$ and $\mathbf{A}_{[\mathbf{range}_k,:]}$.

Attributes

In [83], RESCAL was extended to integrate knowledge about attributes of entities. In this work, the information of attributes of entities was explicitly separated in an additional matrix, but factorized simultaneously with the tensor to couple the latent representations of entities. As discussed in the same work, the attributes could have also been integrated directly into the tensor by treating them as additional entities. Unfortunately, this approach leads to a dramatic increase in size and sparsity of the tensor; the frontal slices would be of shape $(n + a) \times (n + a)$ instead of $n \times n$, where n denotes the amount of entities and a the amount of attributes. Type-constrained RESCAL supports the integration of attributes without any additional adaption of the algorithm, because relations to attributes can be represented as just another type-constrained adjacency matrix $\hat{\mathbf{X}}_{attr}$. By typing these attributes properly (which is the case in schema-based knowledge graphs) and by providing the corresponding type-constraints for datatype properties[5], type-constrained RESCAL can even distinguish different kinds of attributes that might be specific for certain classes of entities.

[5]Datatype properties denote all relation types that relate entities with literals.

Table 5.1: Details on Cora and DBpedia-Music data sets used in the experiments.

Data Set	Entities	Relations	Facts	adjacency tensor $\underline{\mathbf{X}}$
Cora	2,497	10	47,547	2,497 × 2,497 × 10
DBpedia-Music	311,474	7	1,006,283	311,471×311,474×7

5.1.3 Relation to Other Factorizations

The algorithm behind type-constrained RESCAL can be seen as a generalized 2-mode third order tensor factorization methods that contains one global factor matrix for the first and second mode factors. Through this structure, type-constrained RESCAL can mimic other popular 2-mode tensor factorizations very easily. If no type-constraints are available, type-constrained RESCAL transforms into RESCAL. If subject and object entities are not overlapping and the type-constraints for all relation-types are the same, we would get a Tucker2 [105] decomposition. If we have equal range constraints for all relations that are disjunct from the various domain constraints of all relations (which are also disjunct from each other), we would get a similar decomposition as PARAFAC2 [42] (but R_k is not diagonal).

5.1.4 Testing the Integration of Type-Constraints in RESCAL

Below, we will measure the impact of integrating type-constraints into the RESCAL ALS optimization on link-prediction quality and scalability of RESCAL. We conducted link-prediction experiments on two different data sets for this purpose. First, we evaluate against the comparably small Cora[6], which links authors, titles and venues through citation records. For the second data set, we extracted relation-types from the music domain of DBpedia ({*Genre, RecordLabel, associatedMusicalArtist, associatedBand, musicalArtist, musicalBand, album*}. Characteristic dimensions of these data sets can be inferred from Table 5.1.

From each data set, we constructed a partially observed adjacency tensor, where each frontal slice corresponds to the adjacency matrix of one relation-type. We defined the type-constraints based on prior knowledge about the data (Cora) or in case of the DBpedia Data set based on schema information extracted from the corresponding ontology (`rdfs:domain` and `rdfs:range` concepts).

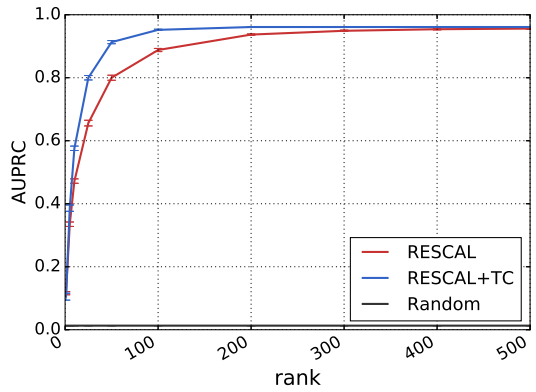
We evaluate the prediction-quality based on link-prediction tasks and measure the

[6]http://alchemy.cs.washington.edu/data/cora/

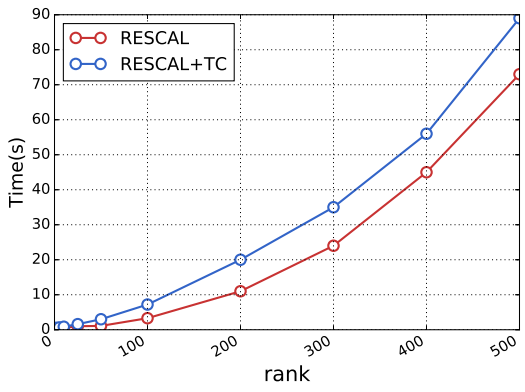
mean Area Under Precision Recall Curve (AUPRC) score after 10 fold cross-validation. For hyper-parameter-tuning and final evaluation, we used the same data and routine for the 10-fold-cross-validation, but we used different seeds for splitting the data into subsets. For the 10-fold cross-validation, we split each data set into 10 random subsets where each subset included observed and unobserved triple which agree with the given type-constraints. In case of the smaller Cora data set, each of these subsets included one tenth of all possible triples sampled from the type-constrained tensor. For the DBpedia-Music data set it is intractable to sample one tenth of the type-constrained tensor due to the huge amount of possible triples. Instead, each of the ten subsets contained one tenth of the observed triples and we randomly sampled 10 times as many unobserved triples and treated them as negative evidence. We made sure that there are no overlaps between the negative evidence of the ten subsets used for cross-validation. In each iteration of the 10-fold cross-validation all true triples contained in one subset are removed from the tensor (set to zero) and the remaining tensor is used for training RESCAL. After training, we predict confidences for all triples contained in this subset and compute the AUPRC for the predicted ranking. We measure and compare the training time in seconds for evaluating the impact of type-constraints on the scalability of RESCAL. As discussed in Section 5.1.2, the integration of type-constraints causes computational overhead, especially when computing the inverses in the update of the factor-matrix $\mathbf{A}$. In case of type-constrained RESCAL, the class-based grouping of entities is included in those measurements. All experiments are conducted with an Intel(R) Xeon(R) CPU W3520 @2.67GHz. In all experiments, RESCAL and Type-Constrained RESCAL were trained for 20 epochs (iterations) of Alternating Least-Squares.

Link-Prediction on Cora

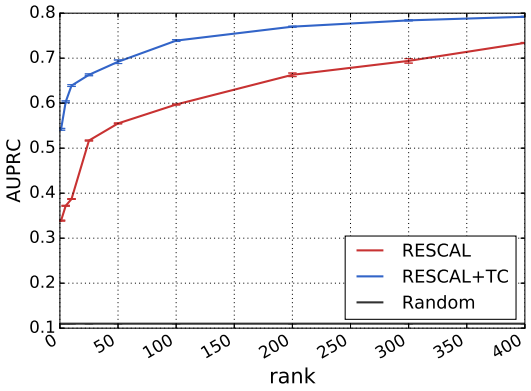
With (RESCAL+TC, blue) and without (RESCAL, red) considering type-constraints, RESCAL performs comparable well on the Cora data set (Figure 5.4.a). Both achieve a maximum score of approx. 0.96 in AUPRC at a rank of 500 (Random: 0.013). By considering type-constraints, it can be observed that the prediction quality increases much faster at lower ranks up to 100. Both approaches achieve similar bad results at a rank of one (0.11 in AUPRC), but for a rank of 25 the integration of type-constraints pays already off, improving the link-prediction quality about 21% in AUPRC from 0.66 to 0.8. At a rank of 100, RESCAL with type-constraints reaches already almost its maximum score of 0.96 whereas the original RESCAL algorithm achieves only 0.89 and needs an four-fold



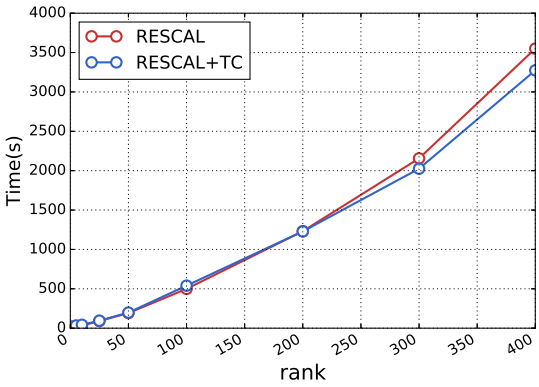
(a) Cora: Rank Vs AUPRC



(b) Cora: Rank Vs Runtime



(c) DBpedia-Music: Rank Vs AUPRC



(d) DBpedia-Music: Rank Vs Runtime

Figure 5.2: Results on the Cora and DBpedia-Music data sets. Shown is the performance of RESCAL with (blue) and without (red) the integration of type-constraints on these data sets. A random ranking is indicated in grey. (a,c) Plotted are the rank used for the factorization against the Area Under Precision Recall Curve (AUPRC) score on the link prediction tasks. (b,d) Shown are the training times in seconds against the rank (dimensionality of the latent embeddings d) used in the factorization

increase in complexity (rank) to achieve the same score.

In Figure 5.4.b we compare the training time of RESCAL in seconds with and without the integration type-constraints. The computational overhead caused by the integration of type-constraints can be clearly seen, but the runtime increases at a very similar pace. Nevertheless, when also considering the link prediction quality measured in AUPRC from Figure 5.4.a, we can argue that the integration of type-constraints results in a low-rank

factorization of much higher quality. Type-constrained RESCAL needs less parameters and less time to achieve good link-prediction results. We already mentioned that by considering type-constraints, RESCAL reaches its maximum performance already at a rank of 100 for which it needs 8 seconds, but without, it needs a four times higher rank of 400 for a similar score leading to a runtime of 57 seconds.

Link-Prediction on DBPedia-Music

The DBpedia-Music data set is considerably larger than the Cora data set and we observe clear differences between RESCAL and its extension (Figure 5.4.c and d). Again, RESCAL with integrated type-constraints (RESCAL+TC) is shown in blue whereas the original algorithm is shown in red. Plotted are the rank of the factorization against the final mean AUPRC (Figure 5.4.c) and the training time in seconds (Figure 5.4.d) after 20 epochs of ALS. The consideration of type-constraints clearly pays of when applying RESCAL to this data set, beating the original approach in terms of AUPRC at any shown rank especially at ranks below 200 (RESCAL: 0.663, RESCAL+TC: 0.770). As observed with the Cora data set, RESCAL's prediction quality starts to catch up at higher ranks and it is expected to hit a comparable performance at some very high rank not covered by the plot. Considering the maximum AUPRC score of the original RESCAL algorithm, which is 0.734 at a rank of 400, by integrating type-constraints into RESCAL this score can already be achieved at a rank of 100. At a rank of 400 it achieves a significantly better score of 0.792.

When comparing the runtime of both methods (Figure 5.4.d), it can be observed that in contrast to the observations for the Cora data set, the training time of both approaches is comparable, but the extended approach starts to slightly outperform the original approach at ranks higher than 300. A reason for this might be that despite the computational overhead generated by integrating type-constraints, the training time seems to benefit from the incorporation of much smaller matrix multiplications in the updates (due to the type-constraints), outweighing the penalty caused by the computational overhead. These size difference between the type-constrained factor matrices ($\mathbf{A}$) becomes more prominent at higher ranks. With increasing rank, these smaller matrices grow much slower in their absolute size than the complete factor matrix $\mathbf{A}$ and therefore the runtime suffers less from an increase in rank (and even compensates for the more complex inverse calculation in the $\mathbf{A}$-updates).

When considering both, the prediction quality and the measured training time, the value of type-constraints for RESCAL becomes even more prominent. RESCAL without

type-constraints reaches an AUPRC score of 0.734 using a rank of 400 after approximately one hour, whereas its extension needed only 9 minutes (rank 100) for the same link prediction quality.

5.1.5 Conclusion

From the results of the conducted experiments an integration of type-constraints as given by the knowledge graph's schema seems very promising. We have seen that despite the computational overhead introduced into RESCAL by integrating type-constraints, the impact on the actual runtime of the algorithm is rather low when RESCAL exploits a similar rank for the factorization. The reason for this lies in the fact that in part the integration of type-constraints results in more efficient computations in the updates. However, by considering that the integration of type-constraints on relation-types results in a better low rank factorization and corresponding embeddings for entities and relation-types, the gained improvements are far more prominent. With the integration of type-constraints, RESCAL is able to achieve similar link-prediction scores at a much lower rank than the original algorithm that ignores type-constraints. This decrease in complexity leads to an order of magnitude lower runtime (seven times on Cora and six times on DBpedia-Music) and model complexity (4 times with both data sets). The better low rank factors are a direct result of the tremendous decrease of the sparsity of the adjacency tensor, allowing type-constrained RESCAL to focus on the correlations and dependencies between real data. We have discussed that RESCAL pushes the learned latent factors to zero if the sparsity of the adjacency tensor is to high, because it primarily focuses fitting the learned function to the overwhelming amount of negative evidence present in the data. The observed benefits in training time and required model complexity are very interesting for modeling large knowledge-graphs, which can only be feasible if we are able to learn meaningful low dimensional latent embeddings for entities and relation-types.

5.2 Type-Constrained Stochastic Gradient Descent

We have seen in the previous section that RESCAL benefits to a large extend from prior knowledge about relation-types in the form of type-constraints as given by the knowledge graph's schema. In this regard, it is especially notable that this prior knowledge has a positive influence on the low dimensional embeddings learned from the data by RESCAL. The integration of schema information is not limited to RESCAL or other ALS optimized

models, but can also be exploited in latent variable models that exploit sampling based optimization algorithms such as stochastic gradient-descent for optimization, i.e. TransE (Chapter 3.3.3) and mwNN (Chapter 3.3.4). One argument for integrating type-constraints into RESCAL is that it decreases the sparsity of the adjacency tensor, thereby avoiding that RESCAL focuses on the overwhelming amount of negative evidence when learning the latent embeddings for entities and relation-types. Sparsity is not an issue in both, TransE and mwNN, because they are optimized through corruption of observed triples. Nevertheless, the corrupted triples are unconstrained, meaning that in large heterogeneous knowledge graphs such as Freebase, large amounts corrupted triples will violate the type-constraints. As a consequence, these algorithms have a strong bias towards learning the difference between type-constraints violating triples and non-violating true triples. In other words the learned latent factors have to additionally explain the type-constraints and therefore higher dimensional embeddings are needed to learn the dependencies between meaningful triples that agree to the sense of the relation-types. In the following subsection, we will describe how the integration of type-constraints can be achieved in TransE and mwNN in more detail. As denoted in Section 5.1.1, for the following sections $\mathbf{domain}_k$ contains the entity indices that agree with the domain constraints of relation-type k and $\mathbf{range}_k$ denotes these indices for the range constraints of relation-type k.

5.2.1 Type-Constrained Triple Corruption in SGD

In contrast to RESCAL, TransE and mwNN are both optimized through mini-batch Stochastic Gradient Descent (SGD), where a small batch of randomly sampled example triples is used in each iteration of the optimization to drive the model parameters to a local minimum. Generally, knowledge graph data does not explicitly contain negative evidence, i.e. false triples[7], and is generated in this algorithms through corruption of observed triples (see Chapter 3.3.3 and 3.3.4). In the original algorithms of TransE and mwNN the corruption of triples is not restricted and can therefore lead to the generation of triples that violate the semantics of relation-types. For integrating knowledge about type-constraints into the SGD optimization scheme of these models, we have to make sure that none of the corrupted triples violates the type-constraints of the corresponding relation-types. We can accomplish this by applying the type-constraints for each sampled true triple (s, p, o) on a set of entities $\mathcal{E}$ from which s' and o' are sampled. For TransE we update Equation 3.4

[7]There are of course undetected false triples included in graph which are assumed to be true.

and get

$$\mathcal{L}^{\mathcal{TC}}_{TransE} = \sum_{(s,p,o)\in T} \sum_{(s',p,o')\in T'} \mathbf{max}\{0, \gamma + \theta_{s',p,o'} - \theta_{s,p,o}\} \tag{5.6}$$
$$\text{with} \qquad s' \in \mathcal{E}_{[\mathbf{domain}_p]} \subseteq \mathcal{E},\ o' \in \mathcal{E}_{[\mathbf{range}_p]} \subseteq \mathcal{E},$$

whereas, in difference to Equation 3.4, we enforce by $s' \in \mathcal{E}_{[\mathbf{domain}_p]} \subseteq \mathcal{E}$ that the subject entities are only corrupted through the subset of entities that belong to the domain and by $o' \in \mathcal{E}_{[\mathbf{range}_p]} \subseteq \mathcal{E}$ that the corrupted object entities are sampled from the subset of entities hat belong to the range of predicate relation-type p. For mwNN, we corrupt only the object entities through sampling from subset of entities $o' \in \mathcal{E}_{[\mathbf{range}_p]} \subseteq \mathcal{E}$ that belong to the range of the predicate relation-type p and get accordingly

$$\mathcal{L}^{\mathcal{TC}}_{mwNN} = -\sum_{(s,p,o)\in T} \log \theta_{s,p,o} - \sum_{o'\in\mathcal{E}_{[\mathbf{range}_p]}\subseteq\mathcal{E}}^{c} \log(1 - \theta_{s,p,o'}) \ . \tag{5.7}$$

In difference to ALS optimized RESCAL, the integration of type-constraints has no direct impact on the update computation as in case of RESCAL, because we apply the constraints only on the triple corruption procedure. The type-constrained sampling of corrupted triples can be realized very efficiently because for any target triple (s, p, o), we simply have to randomly sample entity indices from the precomputed index vectors $\mathbf{domain}_p$ for subject corruption or respectively from $\mathbf{range}_p$ for object corruption. The value of type-constraints for link-prediction with these models will be empirically studied and discussed in Section 5.4.1

5.3 A Local Closed-World Assumption for Modeling Knowledge Graphs

Type-constraints as given by schema-based knowledge graphs tremendously reduce the possible worlds of the statistically modeled knowledge graphs. Unfortunately, type-constraints can also suffer from incompleteness and inconsistency present in the data. Even after materialization, entities and relation-types might miss complete typing, leading to fuzzy type-constraints, leading to disagreements of true facts and present type-constraints in the knowledge graph. For relation-types where these kind of inconsistencies are quite frequent, we cannot simply apply the given type-constraints without the risk of loosing true triples.

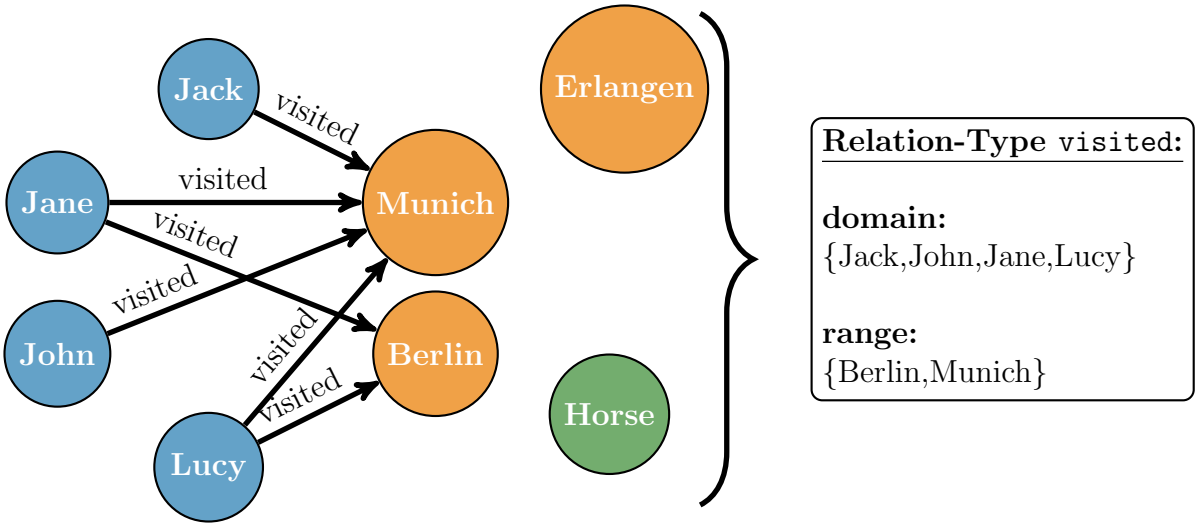


Figure 5.3: Illustration of how the local closed-world assumption is applied to approximate domain and range constraints for a relation-type. The coloring of the nodes indicates which entities would belong to the same class. All person entities (Jack,John,Jane and Lucy) are assigned to the domain of relation-type `visited`, because the graph contains triples where these entities occur as subject. For the range only the cities Munich and Berlin are added and the other entities are excluded from the range, because no relation `visited` has been observed in the graph where they occur as object.

On the other hand, if the domain and range constraints themselves are missing, as e.g. in schema-less KGs, we might consider many triples that do not have any semantic meaning.

We argue that in these cases a local closed-world assumption (LCWA) can be applied, which approximates the domain and range constraints of the targeted relation-type not on class level, but on instance level based solely on observed triples. The idea is shown in Figure 7.1. Given all observed triples, under this LCWA the domain of a relation-type k consists of all entities that are related by the relation-type k as subject. The range is accordingly defined, but contains all the entities related as object by relation-type k. Of course, this approach can exclude entities from the domain or range constraints that agree with the type-constraints given by the RDFS-Schema concepts `rdfs:domain` and `rdfs:range` and the model simply ignores them during model training when exploiting the local closed-world assumption (only for the target relation-type). On the other hand, nothing is known about these entities (in object or subject role) with respect to the target relation-type and therefore treating them as missing can be a valid assumption. In case of the ALS optimized RESCAL, we reduce the size and sparsity of the data by this approach, which has a positive effect on model training compared to the alternative, a closed-world

assumption that considers all entities to be part of the domain and range of the target relation-type [56]. For the stochastic gradient descent optimized TransE and mwNN models, the corruption of triples will result in triples from which we can expect that they do not disagree with the semantics of the corresponding relation-type.

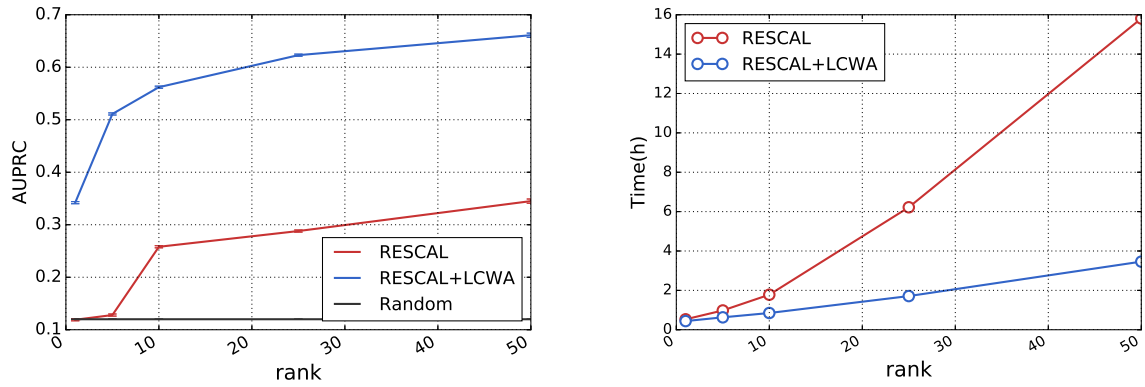
5.3.1 Entity Grouping for RESCAL under a Local Closed-World Assumption

In difference to the type-constraints, which were defined on entity class level, with the local closed-world assumption we deliberately ignore the class membership of entities. As a consequence, we loose the possibility to organize entities in large groups to reduce the amount of inverses that have to be computed in the **A**-updates. We can reduce the amount of different inverses by analyzing the data in a preprocessing step to group entities that share the same pattern of inclusion in the approximated domain and range constraints throughout all relation-types. Nevertheless, in large knowledge graphs where a large amount of relation-types are present and completeness of entities will vary, the grouping will be less successful, resulting in a large amount of small groups. Below, we will empirically study the impact of the local closed-world assumption on the scalability of RESCAL using a large knowledge graph extracted from DBpedia[8] [66]. We extracted all entities with at least five relations and all relation-types that have at least 1000 facts. The resulting graph contained 2,255,018 entities, 511 relation-types and 16,945,046 triples. The corresponding adjacency tensor is of shape 2,255,018×2,255,018×511.

For evaluation and hyper-parameter-tuning we performed 10-fold cross-validation and report the mean Area Under Precision Recall Curve (AUPRC) on a link prediction task. We performed a similar 10-fold cross-validation procedure as used in Section 5.1.4 with the DBpedia-Music data set, only in this case we defined the domain and range constraints based on the local closed-world assumption [9]. We also sampled 10 times as many negative triples from the tensor and ran RESCAL with and without considering the local closed-world assumption for 20 epochs of ALS. The experiment was conducted with an Intel(R) Xeon(R) CPU W3520 @2.67GHz.

[8] http://wiki.dbpedia.org/Downloads39?v=pb8; Data set: Mapping-based Properties (Cleaned)

[9] The domain and range constraints are expected to be not perfectly covering the type-constraints defined by DBpedia's schema, but will suffice to study the impact of the LCWA on RESCAL at this point



(a) DBpedia: Rank Vs AUPRC

(b) DBpedia: Rank Vs Runtime

Figure 5.4: Results on the DBpedia data sets. Shown is the performance of RESCAL with (blue) and without (red) the exploiting the local closed-world assumption on relation-types from the DBpedia Data set. A random ranking is indicated in grey. (a) Plotted are the rank used for the factorization against the score in Area Under Precision Recall Curve (AUPRC) on a link prediction task. (b) Shows the training times in hours with increasing rank used for the factorization.

5.3.2 Link-Prediction in DBpedia with RESCAL

Especially when dealing with a data set of this size (the partially observed tensor is of shape 2,255,018 $\times$ 2,255,018 $\times$ 511), it is important to use models which achieve high prediction quality with low dimensional embeddings, because every additional dimension in the factorization consumes approximately 18 MB of additional memory. We are also dealing with a high amount of relation-types (511), which hardens the grouping of entities. On average we were able to assign the 2,255,018 million entities to approximately 410,000 groups in each training set, thereby decreasing the amount of different inverses per $\mathbf{A}$-update about a factor of five.

With respect to the link-prediction quality, it can be inferred from Figure 5.4.a that due to the sparsity of the tensor (6.52×10^{-9} %) RESCAL (red line in the figure) has problems in capturing the data structure when disregarding any prior assumption on the relation-types, resulting in a factorization of low quality at a very low rank (0.345 AUPRC, rank 50). At a rank of 5 the performance is barely above a random ranking (RESCAL: 0.119, Random: 0.112). As expected and discussed in Section 5.1, we observed that the coefficients in the factor matrices $\mathbf{A}$ and the core tensor $\underline{\mathbf{R}}$ for RESCAL are all very close to zero, meaning that RESCAL indeed tried to fit the overwhelming amount of zeros in

the data.

In comparison, by integrating approximated domain and range constraints (through the local closed-world assumption), better factors that clearly capture structure in the data could be learned at a rank of 5, resulting in an increased link-prediction quality of 0.511 in AUPRC (RESCAL+LCWA, blue line in Figure 5.4.a). Furthermore, at a rank of 50 the factorization starts to become of reasonable quality (0.667)[10] whereas the original algorithm clearly fails (0.345). It can be expected that the original RESCAL will actually achieve similar results when exploiting a sufficiently high rank but, as discussed in Chapter 4, for very large data sets a high rank is intractable or at least a powerful computer system needed.

In Figure 5.4.b, we show the runtime of both RESCAL approaches after 20 epochs of ALS. It can be clearly seen that the training time differences are significantly diverging with higher ranks and the consideration of the approximated domain and range constraints clearly decreases RESCAL's training time. By exploiting the LCWA, the data can be factorized with a rank of 50 in about 3.5 hours (RESCAL+LCWA, AUPRC: 0.667) whereas the original algorithm needs almost 16 hours (RESCAL, AUPRC: 0.345). On a multi-relational data set of this size, where relation-types incorporate only a small subset of entities, the calculations in the updates based on the much smaller factor matrices become very efficient and the larger amount of inverse computations per $\mathbf{A}$-update become insignificant. With increasing rank the gap in training time is expected to increase even further.

5.3.3 Conclusion

Type-constraints of relation-types from schema-based knowledge graphs are not necessarily always present or can be fuzzy. We proposed an alternative local closed-world assumption that can be applied in these cases. This local closed-world assumption approximates domain and range constraints solely based on observed triples in the graph. In case of RESCAL, the approximated domain and range constraints do not consider the class membership of entities and therefore the grouping of entities, which is exploited for decreasing the amount of inverse computations in the $\mathbf{A}$-updates (Section 5.1.2), is less efficient. Based on our experiments on a very large sample from the DBpedia knowledge graph, we were able to show that this drawback is negligible. In fact, we could observe that the local closed-world assumption adds great value to RESCAL, improving runtime

[10] The corresponding Area under ROC curve is 0.84.

and link-prediction quality significantly by exploiting low-dimensional embeddings at the same time.

5.4 Experiments – Prior Knowledge on Relation-Types is Important for Latent Variable Models

In the previous sections, we have shown how prior knowledge about relation-types can be integrated in ALS optimized RESCAL and SGD optimized TransE and mwNN. We showed that in case of RESCAL, domain and range constraints as given by the schema of the knowledge graph or derived by a local closed-world assumption increase the link-prediction quality significantly, if integrated into the optimization algorithm. In this section, we want to study the general value of prior knowledge on the semantics of relation-types for the statistical modeling of knowledge graphs with latent variable models. In the first setting, we assume that curated type-constraints extracted from the knowledge graph's schema are available. In the second setting, we explore the local closed-world assumption proposed in Section 5.3. Our experimental setup covers three important aspects which will enable us to make generalizing conclusions about the importance of such prior knowledge when applying latent variable models to large knowledge graphs:

- We test various representative latent variable models that cover the diversity of these models in the domain. As motivated in the introduction of Chapter 3.3, we belief that RESCAL, TransE and mwNN are especially well suited for this task.

- We test these models at reasonable low complexity levels, meaning that we enforce low dimensional latent embeddings, which simulates their application to very large data sets where high dimensional embeddings are intractable. In [25] for example, the dimensionality of the latent embeddings (d in Chapter 3.3.4) was chosen to be 60.

- We extracted diverse data sets from instances of the Linked-Open Data Cloud, namely Freebase, YAGO and DBpedia, because it is expected that the value of prior knowledge about relation-type semantics is also dependent on the particular data set the models are applied to. From these knowledge graphs, we constructed data sets that will be used as representatives for general purpose knowledge graphs that cover a wide range of relation-types from a diverse set of domains, domain focused

knowledge graphs with a smaller variety of entity classes and relation-types and high quality knowledge graphs.

In tables 5.2,5.3 and 5.4 our experimental results for RESCAL, TransE and mwNN are shown. All of these tables have the same structure and compare different versions of exactly one of these methods on all three data sets. Table 5.2 for example shows the results for RESCAL and Table 5.4 the results of mwNN. The first column in these tables indicates the data sets the model was applied to (Freebase-150k, Dbpedia-Music or YAGOc-195 [11]) and the second column which kind of prior knowledge on the semantics of relation-types was exploited by the model. *None* denotes the original model that does not consider any prior knowledge on relation-types, where *Type-Constraints* denotes that the model has exploited the curated domain and range constraints extracted from the knowledge graph's schema and *LCWA* that the model has exploited the local closed-world assumption (Section 5.3) during model training. The last two columns show the AUPRC and AUROC scores for the various model versions on the different data sets. Each of these two columns contains three sub-columns that show the AUPRC and AUROC scores at different enforced latent embedding lengths: 10, 50 or 100.

Table 5.2: Comparison of AUPRC and AUROC result for RESCAL with and without exploiting prior knowledge about relations types (type-constraints or local closed-world assumption (LCWA)) on the Freebase, DBpedia and YAGO2 data sets. d is representative for the model complexity, denoting the enforced dimensionality of the latent embeddings (rank of the factorization).

RESCAL	**Prior Knowledge on Semantics**	**AUPRC**			**AUROC**		
		$\boldsymbol{d}$=10	$\boldsymbol{d}$=50	$\boldsymbol{d}$=100	$\boldsymbol{d}$=10	$\boldsymbol{d}$=50	$\boldsymbol{d}$=100
Freebase-150k	None	0.327	0.453	0.514	0.616	0.700	0.753
	Type-Constraints	0.521	0.630	0.654	0.804	0.863	0.877
	LCWA	**0.579**	**0.675**	**0.699**	**0.849**	**0.886**	**0.896**
DBpedia-Music	None	0.307	0.362	0.416	0.583	0.617	0.653
	Type-Constraints	0.413	0.490	0.545	0.656	0.732	0.755
	LCWA	**0.453**	**0.505**	**0.571**	**0.701**	**0.776**	**0.800**
YAGOc-195k	None	0.507	0.694	0.721	0.621	0.787	0.800
	Type-Constraints	**0.626**	**0.721**	**0.739**	0.785	0.820	0.833
	LCWA	0.567	0.672	0.680	**0.814**	**0.839**	**0.849**

[11] Details on these data sets are descibed in Section 4.2.1.

Table 5.3: Comparison of AUPRC and AUROC result for TransE with and without exploiting prior knowledge about relations types (type-constraints or local closed-world assumption (LCWA)) on the Freebase, DBpedia and YAGO2 data sets. d is representative for the model complexity, denoting the enforced dimensionality of the latent embeddings.

TransE	**Prior Knowledge on Semantics**	**AUPRC**			**AUROC**		
		d=10	d=50	d=100	d=10	d=50	d=100
Freebase-150k	None	0.548	0.715	0.743	0.886	0.890	0.892
	Type-Constraints	**0.699**	0.797	0.808	**0.897**	0.918	0.907
	LCWA	0.671	**0.806**	**0.831**	0.894	**0.932**	**0.931**
DBpedia-Music	None	0.701	0.748	0.745	0.902	0.911	0.903
	Type-Constraints	**0.734**	0.783	0.826	**0.927**	0.937	0.942
	LCWA	0.719	**0.839**	**0.848**	0.910	**0.943**	**0.953**
YAGOc-195	None	0.793	0.849	0.816	0.904	0.960	0.910
	Type-Constraints	**0.843**	**0.896**	**0.896**	**0.962**	**0.972**	**0.974**
	LCWA	0.790	0.861	0.872	0.942	0.962	0.962

5.4.1 Type-Constraints are Essential

The experimental results shown in Table 5.2, 5.3 and 5.4 give strong evidence that type-constraints as provided by the knowledge-graph's schema are generally of great value to the statistical modeling of knowledge graphs with latent variable models. For all data sets, the prior information on type-constraints significantly improved the link-prediction quality of all models and latent embedding lengths significantly. For RESCAL for example, it can be inferred from Table 5.2 that its AUPRC score on the Freebase-150k data set gets improved from 0.327 to 0.521 at the lowest model complexity ($d = 10$). With higher model complexities the relative improvements decrease, but stay significant (27% at $d = 100$ from 0.514 to 0.654). On the DBpedia-Music data set the improvements are also quite large in AUPRC, e.g. for $d = 10$ from 0.362 to 0.490. In case of the YAGOc-195k data set we only observe large improvements for the lowest model complexity (23% for $d = 10$), but much lower improvements for higher dimensional embeddings with $d = 50$ or $d = 100$ (between 2 to 4% in AUPRC score). The benefit for RESCAL in considering type-constraints was expected due to the results shown in Section 5.1.4 and [17, 56], but the other models show significantly improvements as well when considering type-constraints.

For TransE, we could observe the biggest improvements in case of the Freebase-150k and DBpedia-Music data sets (Table 5.3), where the AUPRC score increases for $d = 10$ from 0.548 to 0.699 in Freebase-150k and for $d = 100$ from 0.745 to 0.826 in DBpedia-

Table 5.4: Comparison of AUPRC and AUROC result for mwNN, the Neural Network model used in [25] with and without exploiting prior knowledge about relations types (type-constraints or local closed-world assumption (LCWA)) on the Freebase, DBpedia and YAGO2 data sets. d is representative for the model complexity, denoting the enforced dimensionality of the latent embeddings.

mwNN	Prior Knowledge on Semantics	AUPRC			AUROC		
		d=10	d=50	d=100	d=10	d=50	d=100
Freebase-150k	None	0.437	0.471	0.512	0.852	0.868	0.879
	Type-Constraints	**0.775**	**0.815**	**0.837**	**0.956**	**0.962**	**0.967**
	LCWA	0.610	0.765	0.776	0.918	0.954	0.956
DBpedia-Music	None	0.436	0.509	0.538	0.836	0.864	0.865
	Type-Constraints	0.509	**0.745**	**0.754**	0.858	**0.908**	**0.913**
	LCWA	**0.673**	0.707	0.723	**0.876**	0.900	0.884
YAGOc-195	None	0.600	0.684	0.655	0.949	0.949	0.957
	Type-Constraints	**0.836**	**0.840**	**0.837**	**0.953**	**0.954**	**0.960**
	LCWA	0.714	0.836	0.833	0.926	0.935	0.943

Music. Also, in case of the YAGOc-195k data set the link-prediction quality could be improved from 0.793 to 0.843 with $d = 10$.

Especially the multiway neural network approach (mwNN) seems to improve the most by considering type-constraints for relation-types into the model (Table 5.4). For Freebase-150k, we observe improvements up to 77% in AUPRC for $d = 10$ from 0.437 to 0.775. On the DBpedia-Music data set, the type-constraints improve mwNN from 0.436 to 0.509 ($d = 10$) and from 0.538 to 0.754 in AUPRC ($d = 100$). In case of the YAGOc-195k data set the approach with type-constraints is also clearly superior.

Besides observing that the latent variable models are superior when exploiting type-constraints at a fixed latent embedding dimensionality d, it is worth noticing that the biggest improvements are most often achieved at the lowest model complexity ($d = 10$), which is especially interesting for the application of these models to very large data sets. At this low complexity level the type-constraint supported models even outperform more complex counterparts that ignore type-constraints, e.g. on Freebase-150k mwNN reaches 0.512 AUPRC with an embedding length of 100 but by considering type-constraints this models achieves 0.775 AUPRC with an embedding length of only 10.

5.4.2 Local Closed-World Assumption – Simple but Powerful

In Section 5.4.1 we have declared based on empirical results that type-constraints are very important for the statistical modeling of knowledge graphs with latent-variable models. Unfortunately, type-constraints are not always available or can be fuzzy for some relation-types due to incompleteness of the underlying knowledge graph. The local closed-world assumption (LCWA) discussed in Section 5.3 offers an alternative in these cases because it relies solely on observed triples.

It can be observed from tables 5.2, 5.3 and 5.4 that similar to the type-constraints, the approximation of domain and range constraints through the Local Closed-World Assumption generally leads to large improvements in link prediction results over the same models that do not consider any prior knowledge about relation-types, especially at the lowest model complexities ($d = 10$). For example, TransE gets improved from 0.715 to 0.806 with $d = 50$ in the Freebase-150k data set, mwNN improves its initial AUPRC score of 0.600 ($d = 10$) on the YAGO data set to 0.714 and RESCAL's AUPRC score jumps from 0.327 to 0.579 ($d = 10$). The only exception to these observation is RESCAL when applied to the YAGOc-195k data set. For $d = 50$, RESCAL's AUPRC score decreases from 0.694 to 0.672 and for $d = 100$ from 0.721 to 0.680 when considering the LCWA in the model. The type-constraints of the relation-types in the YAGOc-195 data set are defined over a large set of entities (we evaluate on the type-constrained knowledge graph). When applying type-constraints to the YAGOc-195k data set, 22% of all possible triples are covered. It seems that a closed-world assumption is more beneficial for RESCAL than a LCWA in this case.

Even though the LCWA has a similar strong impact on link-prediction quality than the curated type-constraints, there is no evidence in our experiments that the LCWA can generally replace the semantic prior knowledge about entity types and type-constraints on relation-types given by the schema of the knowledge-graph. For the YAGOc-195k data set the AUPRC scores for the models that exploit the LCWA are often clearly worse than their counterparts that use the type-constraints extracted from the knowledge graph. TransE with type-constraints achieves an AUPRC score of 0.896 whereas LCWA supported TransE reaches only 0.861 with an embedding length of 50. For $d = 10$, mwNN with type-constraints reaches an AUPRC score 0.836 whereas the application of the LCWA leads only to 0.714.

In case of the other two data sets the message is not as clear. RESCAL achieves its best results when exploiting LCWA instead of type-constraints, whereas TransE shows

better performance only for latent embeddings of length 50 and 100 but not with a length of 10. For $d = 100$, the combination of TransE and the LCWA improves the AUPRC score to 0.831 (0.808 with type-constraints) in Freebase-150k and 0.839 (0.783 with type-constraints) in DBpedia-Music. At the lowest model complexity ($d = 10$) on the other hand, the integration of type-constraints is superior over the LCWA.

For mwNN the observations are the opposite to those of the TransE extensions in case of DBpedia-Music. In case of the Freebase-150k data set the integration of the extracted type-constraints is always clearly better, reaching 0.815 in AUPRC with an embedding length of 10 (0.765 with LCWA).

5.5 Related Work

A general overview on the related work in the field of statistical modeling of knowledge graphs with latent variable models is provided in Chapter 4.4. Integrating domain and range constraints as given by the knowledge graph's schema into RESCAL has also been proposed by [17]. Local closed-world assumptions are a known concept in the semantic web domain [96]. The neural network approach used in the Google Knowledge Vault System, in this work denoted as mwNN, also exploits a local closed-world assumption for corrupting triples (negative sampling). As described in Chapter 3.3.4, this local closed-world assumption only excludes unobserved subject entities from the negative sampling. In difference to the local closed-world assumption used in this chapter, the object entity of an observed triple can be corrupted through any entity present in the knowledge graph.

In case of RESCAL, prior information on type-constraints can also be integrated by the method proposed in [69], which introduced a weighted loss functions for RESCAL. Via such loss functions relational type-constraints are integrated in the RESCAL optimization by assigning zero weights to triples that are excluded through type-constraints. Unfortunately, the scalability of RESCAL gets lost when using this type of weighted loss function. The Hadamard (element wise) matrix product with the weighting tensor leads to expensive matrix operations in the gradients, since a materialization of a complete frontal slice reconstructed from the learned latent representation of the data is required (the product AR_kA^T), which is dense. Besides the high computational costs that arise during this materialization in the gradient, the memory requirements for this materialization itself will be extensive which makes this approach impractical for large knowledge graphs. For example, consider the music domain of DBPedia (321,950 entities). The materialization of

a single frontal slice (AR_kA^T) will need approximately 829 GB of memory (considering double precision floats).

5.6 Conclusion

In this chapter, we have motivated and studied the general value of prior knowledge about the semantics of relation-types extracted from the schema of the knowledge-graph (type-constraints) or approximated through a local closed-world assumption for the statistical modeling of knowledge graphs with latent variable models. We have shown that this prior knowledge can be integrated in the ALS optimized RESCAL, but also in the SGD optimized TransE and mwNN models without sacrificing the scalability of these models. Our experiments give clear empirical proof that the curated semantic information of type-constraints significantly improves link-prediction quality of TransE, RESCAL and mwNN (up to 77%) and can therefore be considered as essential for latent variable models when applied to large knowledge graphs. In this regard, the value of type-constraints becomes especially prominent when the model complexity, i.e. the dimensionality of the embeddings, has to be very low which is an essential requirement when applying these models to very large data sets.

Since type-constraints are not always present or can be fuzzy (due to e.g. insufficient typing of entities) we further showed that an alternative, a local closed-world assumption (LCWA), can be applied in these cases that approximates domain and range constraints on instance rather on class level solely based on observed triples. This LCWA leads to similar large improvements in the link-prediction tasks than the type-constraints, but especially at a very low model complexity the integration of type-constraints seemed superior. In our experiments we used models that either exploited type-constraints or the LCWA, but in a real setting we would combine both, where type-constraints are used whenever possible and the LCWA in case type-constraints are absent or fuzzy.

Chapter 6

Ensemble Solutions for Representation Learning in Knowledge Graphs

We have motivated in Chapter 3.3 that RESCAL[82], TransE [9] and the multiway neural network proposed in [25] (mwNN) represent the diversity of state of the art latent variable models for the statistical modeling of knowledge graphs. In the last chapter, we have shown that these models can be improved individually by integrating prior knowledge about relation-types in form of type-constraints or derived through a local closed-world assumption. In this regard and in Chapter 4.3, we could observe that these models also differ in their link-prediction capabilities when applied to large knowledge graphs under realistic settings. A large amount of literature is putting a lot of effort in finding the best model for a certain use-case in the context of knowledge graphs, e.g. link-prediction, selling the proposed method as the superior overall model. From our opinion, it is often disregarded that these models might model different aspects of the data and therefore even models with lower prediction quality are able to contribute non redundant dependencies learned from the data. In all of our experiments, TransE often significantly outperformed the other two methods on the tested data sets in link-prediction tasks, but we argue that all three methods are substantially different in multiply aspects regarding their modeling assumptions and technical details and therefore chances are high that they learn different patterns in the data that can be complemented. In this chapter, we study the complementary potential of these models by combining them in very simple ensembles. We also consider type-constraints and the local closed-world assumption in the individual models, due to their importance for the statistical modeling of knowledge graphs (see Chapter 5). Based on the conducted experiments on multiple datasets, we show that TransE's link

predictions are complemented by predictions made by RESCAL and mwNN.

The content of this chapter is completely covered in:

[58] Denis Krompaß and Volker Tresp. *Ensemble Solutions for Representation Learning in Knowledge Graphs* ECML Workshop on Linked Data for Knowledge Discovery. 2015

6.1 Studying Complementary Effects between TransE, RESCAL and mwNN

The main characteristic of a good ensemble is its composition out of very diverse single predictors that learn and recognize different patterns in the data. Through the diversity of the different predictors often complementary effects can be observed that drive overall prediction quality. As discussed in chapter 3.3, there is a large diversity between RESCAL, TransE and mwNN. RESCAL assumes normally distributed variables minimizing a least-squares loss function, whereas mwNN assumes Bernoulli distributed variables minimizing a logistic loss function. TransE on the other hand minimizes a max-margin based ranking loss function. Furthermore, RESCAL is a third-order tensor factorization method that is optimized through alternating least-squares, whereas TransE is a distance based model and mwNN a neural network that are both optimized through stochastic gradient-descent combined with negative sampling. In addition, mwNN and TransE differ in the way they corrupt triples for the negative sampling. In TransE, two corrupted triples are sampled for each true triple, where in each corrupted triple the subject or object entity is replaced (but never at the same time). mwNN generates negative triples by only corrupting the object entities with randomly sampled entities. In difference to the other methods, TransE does not include any regularization besides enforcing an L2-norm of 1 for the latent embeddings of the entities. RESCAL uses a L2 regularization and we minimized mwNN with elastic net regularization and additional DropConnect [111] on the network weights.

For our study, we build simple ensembles in which we combine the link-predictions of RESCAL, TransE and mwNN. The final probability of a triple is then derived from the

combination of these predictions by

$$P(x_{s,p,o}=1|\Theta) = \frac{1}{n}\sum_{\theta^m\in\Theta}^{n} P(x_{s,p,o}|\theta^m_{s,p,o}) \quad (6.1)$$

$$\text{where} \quad \Theta \subseteq \{\theta^{RESCAL}, \theta^{TransE}, \theta^{mwNN}\}$$

$$\text{and} \quad P(x_{s,p,o}=1|\theta^m_{s,p,o}) = \frac{1}{1+\exp\{-(\omega^m_1\theta^m_{s,p,o}+\omega^m_0)\}} \quad (6.2)$$

$$\text{with} \quad \theta^{RESCAL}_{s,p,o} = \mathbf{a}_s^T\mathbf{R}_p\mathbf{a}_o \text{ (Equation 3.2)},$$

$$\theta^{TransE}_{s,p,o} = -\delta(\mathbf{a}_s+\mathbf{r}_p,\mathbf{a}_o) \text{ (Equation 3.3)},$$

$$\theta^{mwNN}_{s,p,o} = \sigma(\beta^T\phi(\mathbf{W}[\mathbf{a}_s,\mathbf{r}_p,\mathbf{a}_o])) \text{ (Equation 3.5)},$$

where $x_{s,p,o}$ is the target variable that indicates if a triple (s,p,o) consisting of the subject and object entities s and o and the predicate relation-type p is true.

Θ holds the pool of model parameters the ensemble combines for the prediction. We are evaluating all possible combinations of models, therefore Θ can be just a subset of the three, RESCAL, TransE and mwNN. For the ensemble, we train and find the best hyper-parameters for each model θ^{RESCAL}, θ^{TransE} and θ^{mwNN} independently, but the predicted confidence scores for triples generally differ between all model; mwNN predicts values between 0 and 1, whereas RESCAL can return any value in $\mathbb{R}$ and TransE returns negative distances. We could have applied a simple meta-learner, e.g. a simple logistic regression or a feed-forward neural network with one hidden layer to auto-balance the outputs of the tree methods, but we expected that such a meta learner could blur the individual contribution of each single-predictor in the link-prediction tasks. Instead, we use a Platt-Scaler [87] for each model based on a small subsample of the training data to get properly scaled probabilities (Equation 6.2). A Platt-Scaler is basically a logistic regression model that takes exactly one input (the output $\theta^m_{s,p,o}$ of the model m) and maps it to the interval $[0,1]$. The scalars ω^m_1 and ω^m_0 in Equation 6.2 denote the learned weight and bias of the logistic regression (Platt-Scaler) for the model m.

In difference to the other two methods, mwNN already predicts probabilities for triples. Nevertheless, we also learned a Platt-Scaler for this model in order to calibrate the probabilities of all models on the same data set. For the final probability of a triple (s,p,o), we apply the scalers to the confidence score $\theta^m_{s,p,o}$ of each model m to get the probability $P(x_{s,p,o}|\theta^m_{s,p,o})$, that is the probability of the triple (s,p,o) given the model m. Subsequent to that, we simply combine each of these probabilities by computing the arithmetic mean (Equation 6.1).

6.2 Experimental Setup

With our experiments we study if TransE, RESCAL and mwNN are good targets for combination to drive link-prediction quality. We will further check if one model is not contributing any additional knowledge to the ensemble by evaluating ensembles where only two of the three models are combined. The above two steps are evaluated in two settings, where in the first setting the models are exploiting type-constraints extracted from the knowledge-base schema and in the second setting they solely use the local closed-world assumption (LCWA) proposed in Chapter 5.3. With the second setting we check if LCWA based models are also learning complementary information. As discussed in chapter 5.3 the LCWA has the benefit that it can be exploited without the need of prior knowledge about the types of the entities and the typing of the relation-types. Therefore they can be applied to single relation-types or whole knowledge-graphs where information about type-constraints is absent or fuzzy. We evaluate the different ensembles on link-prediction tasks, using the same data sets (Freebase-150k, Dbpedia-Music, YAGOc-195k) and evaluation procedure as described in Chapter 4.2.1 and 4.2.2. The ensembles were also implemented in python using the code of RESCAL, TransE and mwNN, which has been described in Chapter 4.2.3. After hyper-parameter tuning we retrained all models using the best hyper-parameters on the validation and training set and used 5% of this combined training set for learning the Platt-Scalers for each model (RESCAL, TransE and mwNN). We report the Area Under Precision Recall Curve (AUPRC) score for each ensemble and in addition we report the AUPRC for the best single predictor as comparison.

6.3 Experiments – TransE, RESCAL and mwNN Learn Complementary Aspects in Knowledge Graphs

In Table 6.1 the AUPRC results on the extracted data sets from Freebase, YAGO and DBpedia for the first setting are shown, where all models exploit the type-constraints given by the RDF-Schema concepts. Table 6.2 shows the same for the second setting where the models solely exploited the Local Closed-World Assumption. *ALL* represents the ensemble consisting of TransE, RESCAL and mwNN and the beneath three models represent the ensembles that combine all possible pairs of models, e.g. mwNN + TransE represents the ensemble consisting of mwNN and TransE. *Best Single Predictor* represents the best model out of TransE, RESCAL or mwNN on the same link-prediction task. Which of the three

Table 6.1: AUPRC results on data sets, exploiting **Type-Constraints** in the models. **Model←*d*** indicates the dimensionality of the latent embeddings used by the models.

Model←*d*=10	Freebase@100	DBpedia-Music	Yago-Core@5
ALL	**0.846**	0.815	**0.883**
mwNN + TransE	0.820	**0.817**	0.881
mwNN + RESCAL	0.795	0.519	0.821
TransE + RESCAL	0.757	0.748	0.859
Best Single Predictor	(mwNN) 0.775	(TransE) 0.734	(TransE) 0.843

Model←*d*=50	Freebase@100	DBpedia-Music	Yago-Core@5
ALL	**0.892**	**0.827**	**0.902**
mwNN + TransE	0.876	0.825	0.900
mwNN + RESCAL	0.835	0.756	0.845
TransE + RESCAL	0.819	0.783	0.891
Best Single Predictor	(mwNN) 0.815	(TransE) 0.783	(TransE) 0.896

Model←*d*=100	Freebase@100	DBpedia-Music	Yago-Core@5
ALL	**0.904**	**0.843**	**0.911**
mwNN + TransE	0.893	0.842	0.909
mwNN + RESCAL	0.852	0.762	0.862
TransE + RESCAL	0.826	0.825	0.901
Best Single Predictor	(mwNN) 0.837	(TransE) 0.826	(TransE) 0.896

models had the best AUPRC score is shown in the brackets next to the corresponding score in that row. d is the chosen dimensionality of the embeddings or the rank of the factorization in case of RESCAL (e.g. $Model \leftarrow d = 100$ indicates that all models were trained with a fixed embedding dimensionality of 100).

6.3.1 Type-Constrained Ensembles

From Table 6.1, it can be observed that the ensemble consisting of all three models (with type-constraints) is clearly outperforming the best single predictor on all data sets and with all different embedding dimensions (10,50,100). On the Freebase-150k data set, we see the biggest improvements with an embedding length of 10 and the ensemble increases the AUPRC score from 0.775 to 0.846 in this case. For $d = 100$ the score improves form 0.837 to 0.904 in AUPRC. In the other two data sets we observe large improvements for the lowest embedding dimensionality of 10 (11% on DBpedia-Music and 5% on YAGOc-195k), but for higher dimensional embeddings ($d = 50$ and $d = 100$) the improvements are

decreasing or vanishing (YAGOc-195k).

The improvements observed for the really low embedding vector dimensionality of 10 are of special interest. As discussed in Chapter 4, in a Web-Scale application of these algorithms it is of high interest to have meaningful embeddings in a very low dimensional latent space because higher dimensional representations can lead to long or even intractable runtimes for model training and tuning. It can be observed that the ensemble consisting of TransE, RESCAL and mwNN with a embedding length of 10 reaches comparable link prediction results than the best single predictor with an embedding vector length of 100. On the Freebase-150k data set the ensemble reaches an AUPRC score of 0.846, on DBpedia-Music 0.815 and YAGOc-195k 0.883 with $d = 10$, whereas the best single predictor reaches 0.837, 0.826 and 0.896, respectively, with $d = 100$.

When it comes to the contribution of each single predictor to the ensemble, we observe that in case of the Freebase data set all models are contributing to the superior performance of the ensemble, but TransE and mwNN are responsible for the biggest increase in AUPRC. For example, with $d = 10$ TransE+mwNN achieves an AUPRC of 0.820 whereas mwNN+RESCAL reaches 0.795 and TransE+RESCAl 0.757. On the DBpedia-Music and YAGOc-195k data set, RESCAL does not add any significant value to the ensemble, e.g. for $d = 50$ mwNN+TransE have the highest AUPRC score of the pairwise ensembles reaching already 0.825 on DBpedia-Music and 0.900 on YAGOc-195k, whereas the maximum performance of the complete ensemble (ALL) lies at 0.827 and 0.902.

As a final remark we could observe from the results shown in Table 6.1 that RESCAL or mwNN best complement with TransE. The combination of mwNN and RESCAL generally shows less improvements in AUPRC compared to the best single predictor performance of those two (compare with Tables 5.2, 5.3 and 5.4), indicating that these two models learn more similar patterns from the data.

6.3.2 Ensembles under a Local Closed-World Assumption

The results for the LCWA ensemble are shown in Table 6.2. We see the largest improvements on the Freebase-150k data set, where the ensemble improves the AUPRC score compared to the best single predictor from 15% ($d = 10$) to 9% ($d = 100$). Also, all predictors (RESCAL,TransE, mwNN) contribute to the performance of the ensemble, since all ensembles consisting of two models achieve a significantly lower AUPRC score in this case. The highest pair-ensemble (TransE + RESCAL) achieves 0.763 ($d = 10$), 0.876 ($d = 50$) and 0.899 ($d = 100$) whereas the full ensemble achieves 0.775, 0.886 and 0.909. On the

Table 6.2: AUPRC results on data sets, exploiting the **Local Closed-World Assumption** in the models. **Model←*d*** indicates the dimensionality of the latent embeddings used by the models.

Model←*d*=10	Freebase@100	DBpedia-Music	Yago-Core@5
ALL	**0.775**	**0.787**	**0.825**
mwNN + TransE	0.729	0.780	0.820
mwNN + RESCAL	0.649	0.661	0.679
TransE + RESCAL	0.763	0.746	0.806
Best Single Predictor	(TransE) 0.671	(TransE) 0.719	(TransE) 0.790

Model←*d*=50	Freebase@100	DBpedia-Music	Yago-Core@5
ALL	**0.886**	**0.841**	**0.899**
mwNN + TransE	0.854	**0.841**	0.890
mwNN + RESCAL	0.820	0.661	0.828
TransE + RESCAL	0.876	0.746	0.878
Best Single Predictor	(TransE) 0.806	(TransE) 0.839	(TransE) 0.861

Model←*d*=100	Freebase@100	DBpedia-Music	Yago-Core@5
ALL	**0.909**	0.844	**0.900**
mwNN + TransE	0.884	0.844	0.890
mwNN + RESCAL	0.852	0.734	0.847
TransE + RESCAL	0.899	0.845	0.886
Best Single Predictor	(TransE) 0.831	(TransE) **0.848**	(TransE) 0.872

DBpedia-Music data set the ensemble only improves the best single predictor for very low dimensional embeddings ($d = 10$) from 0.719 to 0.787. For a embedding vector length of 50 and 100 the ensemble does not improve the best single predictor in this data set. The ensemble constantly improves the best single-predictor on the YAGOc-195k data set of about 0.03 to 0.04 in AUPRC for all embedding vector lengths. We also see a small improvement of the full ensemble opposed to the best ensemble consisting of TransE and mwNN. As in case of the type-constrained ensembles, we can also observe from Table 6.1, that mwNN and RESCAL best complement with TransE.

6.4 Related Work

The related work on the statistical modeling of knowledge graphs is described in Chapter 4.4 and the integration of prior knowledge about relation-types in Chapter 5.5. There

has been little amount of work on combining latent variable models for link-prediction in knowledge graphs. Very recently, [36] combined two independent models of different complexity in an ensemble (TATEC) to improve link-prediction. As in [99] a three-way model is combined with a two-way model in this case, but in TATEC the two models are trained independently and combined later. [43] used a bagging approach to combine various classification algorithms (e.g. Support-Vector-Machines, K-Nearest-Neighbor) for link-prediction, but could not observe any significant improvements over the best single predictors.

6.5 Conclusion

In this work we showed that the the predictions of three leading latent variable models for link-prediction in large knowledge-graphs are indeed complementary to each other and can be exploited in an ensemble solution to improve overall link-prediction quality. We observed in our experiments that especially TransE learns substantially different aspects of the data than RESCAL and mwNN. RESCAL and mwNN on the other hand are more similar to each other, even though these two models differ in various aspects. We further showed that an ensemble consisting of all three methods brings substantially higher prediction quality on all used data sets and all settings when the models need to exploit a very low dimensional embedding space ($d = 10$). The LCWA can also be exploited in the ensemble when the type-constraints for properties are absent or fuzzy. On the DBpedia-Music and YAGOc-195 data set we observed that with a higher dimensional latent embedding space the improvements become less significant.

Chapter 7

Querying Statistically Modeled Knowledge Graphs

It is a known fact that the Web of Data is fairly incomplete and contains incorrect information, as triples are missing and existing triples can be false. Generally, information in the form of triples extracted from such data is afflicted with uncertainty that is persistent in the source data, has been introduced by human curators or information extraction methods. In many cases, the valuable information about uncertainty is discarded and some threshold is applied to filter more probable triples, which is dependent on the extraction technique applied. When accessing these data sets, we typically only see what is left after this pruning step and the information about the uncertainties is irreparably lost.

In the previous chapters, we have shown that latent variable models are powerful models that are especially well suited for the statistical modeling of knowledge graphs and that generate confidence values for observed and unobserved triples which can be exploited for the completion and cleansing of knowledge graphs. In other words, these models reintroduce a measure of uncertainty into the graph that represents the beliefs of the model into observed and unobserved triples derived from the learned dependencies in the data. Applying latent variable models for link-prediction tasks can be seen as querying these models for ground triples to derive probabilities that describe the likelihood of their occurrences over the vast amount of possible deterministic instantiations (worlds) of the graph. Probabilistic databases (PDBs) naturally consider multiple possible instances of a database via the possible worlds semantics and account for uncertainty in the data by assigning a probability distribution over all of these database instances [100]. As a conclusion, we could interpret the statistically modeled knowledge graph as a probabilistic database, where the

latent variable model is defining the underlying probability distribution of triples. As such, we could proceed and exploit these modeled graphs for complex querying that goes beyond the querying of ground triples. Querying probabilistic databases has a clear interpretation as generalization of deterministic relational database querying.

When applying PDBs to large triple stores, various key challenges need to be addressed. First, we have to consider storage requirements. A common assumption in PDBs is tuple independence, or in our case triple independence, which requires a representation of each triple's uncertainty. Unless default values are used, representing the individual uncertainty levels can lead to huge storage requirements.

Second, probabilistically correct and efficient querying. Although individual triples are assumed to be independent, complex queries introduce dependencies such that correct query answering becomes, in the worst case, intractable.

These two challenges are intertwined, since we cannot explicitly represent the uncertainty values of all possible triples, and the generation of these uncertainties "on the fly" during query evaluation can introduce intractable evaluation complexity.

In this chapter, we will address these issues by exploiting intrinsic features of latent variable models, i.e. RESCAL, TransE and mwNN, when evaluating safe queries on probabilistic knowledge graphs derived from these models.

This chapter is structured as follows: In the next section, we will give an introduction to the theory of probabilistic databases and extensional query evaluation, which is used for evaluating safe queries. In Section 7.2, we will discuss how latent variables can be exploited for probabilistic querying of statistically modeled knowledge graphs. We will further describe how the efficiency of query evaluation can dramatically improved by exploiting intrinsic features of these models. Subsequent to that, we will empirically analyze the proposed approach based on RESCAL in Section 7.3 and 7.4. We provide related work in Section 7.5 and conclude in Section 7.6.

A large part of the contributions covered in this chapter are published in:

[57] Denis Krompaß, Maximilian Nickel and Volker Tresp. Querying Factorized Probabilistic Triple Databases. Proceedings of the 13th International Semantic Web Conference (ISWC, Best Research Paper Nominee), 2014.

In addition, this chapter includes various extentions to the content published in [57]:

1. We describe how compound relations can also be learned with TransE [9] and the multiway neural network (mwNN) [25] in Section 7.2.

2. For the learning of compound relations type-constraints were considered by RESCAL [82], TransE and mwNN as described in Chapter 5 in both, the methodology (Section 7.2) and experiments (Section 7.3 and 7.4).

3. We included a brief discussion on the numerical advantages of learned compound relations in the context of extensional query evaluation rules in Section 7.2.3.

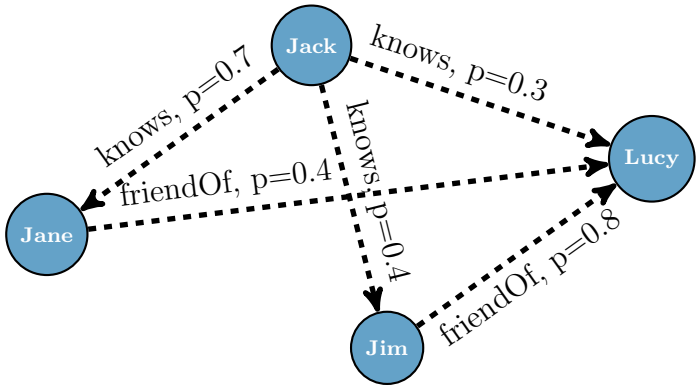
4. We conducted more extensive experiments in Section 7.3, evaluating the proposed approach based on all possible compound relations that could be constructed from the UMLS and Nations datasets.

5. The DBpedia-Music Dataset has been extracted from the more recent DBpedia release DBpedia2014.

6. In addition to the area under receiver characteristic (AUROC) which we used in [57] to analyze the ranking of the returned answers after the probabilistic querying of factorized DBpedia-Music (Section 7.4), we also report the area under precision recall curve (AUPRC) for a better analysis of the ranking of these answers and the logloss score to analyze and discuss the quality of the generated probabilities associated with these answers.

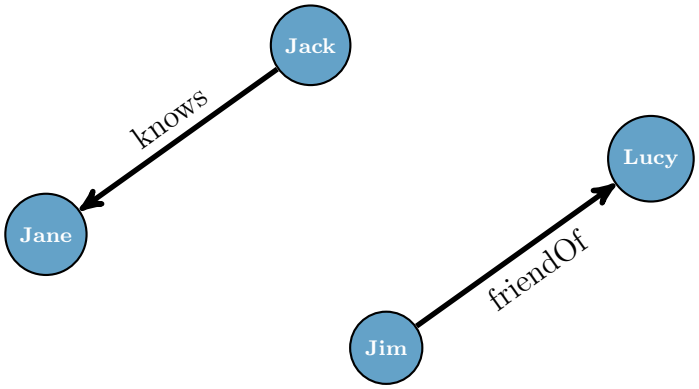
7.1 Exploiting Uncertainty in Knowledge Graphs

Knowledge graphs are generally deterministic representations of world knowledge, i.e. triples, but in reality only represent one possible instantiation of the graph that has been derived from a large set of partially uncertain triples. Uncertainties naturally occur with triples for multiple reasons. The uncertainty of a contribution might reflect the confidence of a human contributor into the added fact, which might in turn depend on the level of expertise of the contributor. This uncertainty is rather low in small graphs that are built by a small group of experts, whereas it increases in larger graphs where in principle every human can contribute. Automated information extraction methods such as NELL naturally generate probabilities when performing e.g. relation extraction from unstructured texts. Also rule based approaches as used in DBpedia or YAGO lead to extraction of triples that introduce some degree of uncertainty into the data. Uncertainty can also be dependent on the source of information. Knowledge graphs such as Freebase include triples from different sources, where these sources themselves vary in reliability.



Extracted Triples	p
(Jack,knows,Jane)	0.7
(Jack,knows,Jim)	0.4
(Jack,knows,Lucy)	0.3
(Jane,friendOf,Lucy)	0.4
(Jim,friendOf,Lucy)	0.8

(a) Raw triples provided by a hypothetical information extraction pipeline



Remaining Triples	p
(Jack,knows,Jane)	1.0
(Jim,knows,Lucy)	1.0

(b) Graph left after pruning the graph in (a) with $p \geq 0.5$

Figure 7.1: Illustration of a knowledge graph before (a) and after (b) transforming and filtering the extracted triples based on uncertainty.

In most of the cases, a post processing step is performed on these triples, thereby discarding the uncertainties by including only triples with a sufficient certainty level. In Google's Knowledge Vault only triples with a certainty above 0.9 are included and the rest is discarded. Generally, valuable information is hidden in the uncertainty of triples, even by those with a large uncertainty. This can be exemplified by considering the hypothetical set of extracted triples and corresponding graph shown in Figure 7.1a. This graph consists of four person entities (`Jim`, `Jane`, `Jack`, `Lucy`), two different kinds of relationships (`friendOf`, `knows`) and we are also provided with the probabilities of these triples. Not all of these triples have a very high probability, e.g. $(\texttt{Jack}, \texttt{knows}, \texttt{Lucy}), p = 0.3$. In general, triples with low probabilities are pruned out of the knowledge graph based on some threshold. In Figure 7.1b this is exemplified based on a threshold of 0.5[1]. The remaining triples are considered to be correct and the probabilities are discarded, thereby transforming the set of uncertain triples into a deterministic database (or graph). A simple query on each of these two graphs (Figure 7.1a and b) illustrates the impact on information loss of such an approach. Let us consider the query $\exists y.(knows(\texttt{Jack}, y), friendOf(y, \texttt{Lucy}))$ that asks if the entity Jack knows someone who is a friend of Lucy. Asking this query on the pruned deterministic database instance will result in no answer because there is none such person in the database. On the other hand, if we would exploit all initial triples with their probabilities, we could infer that there is such a person with a fairly high probability of 0.66[2], which is higher than the threshold used for the pruning. In order to exploit the valuable information that is provided by the uncertainty of triples and its potential, a database system must be able to understand and process triples with their probabilities. Next, we will give some basic background on the theory of probabilistic databases, which allow probabilistic inference from uncertain data for processing and answering database queries. The theory of probabilistic databases offers a system to exploit probabilities of triples for probabilistic inference in order to compute query answers.

7.1.1 Notation

In the following sections we exploit the syntax of non-recursive datalog rules for queries of the form

$$Q(x, z) :- L_1(x, y), L_2(y, z)$$

[1] In a real setting, a much higher threshold is used.

[2] This probability can be simply computed through the independent-project rule (Equation 7.5); we assumed that any person knows and is a friend of itself.

where $Q(x, y)$ is the head of the rule of query Q with head variables x and y. $L_1(x, y), L_2(y, z)$ is the body of the rule consisting of a conjunction (denoted by the ",") of the two relational atoms L_1 and L_2. As generally used in relational calculus, $\vee$ and $\wedge$ will denote a logical disjunction and conjunction, respectively. Further $\exists y$ will denote the existential quantifier for the variable y. The *active domain ADom* of a database is the set of all constants occurring in the database. $Q[\bar{a}/\bar{x}]$ represents the query where the variable $\bar{x}$ has been substituted by the constants $\bar{a}$ where $\forall a \in \bar{a} : a \in ADom$. Further, $DomX$ is the domain of a random variable X; the set of values that can be assigned to X. Φ will denote a propositional formula consisting of disjunctions, conjunctions and negation (denoted as $\neg$) of random variables. As used in set theory we will denote the union of two sets as $\bigcap$ and express a subset dependency of two sets as $\subseteq$. We will interchangeably use the notation (s, p, o) or $p(s, o)$ to represent triples, where the latter notation is also referred to as relational tuple. In that context, p indicates the predicate relation-type and s and o are the subject and object entities, respectively.

7.1.2 Probabilistic Databases

Probabilistic databases (PDB) have been developed to extend database technologies to handle uncertain data. A general overview is provided by [100]. PDBs build on the concept of incomplete databases, which, in contrast to deterministic databases, represent multiple possible instances (worlds) of a database. One example how these multiple worlds can emerge is by looking at mutual exclusive relations as the e.g. `birthplace` relation-type. Obviously, a person can only have one birthplace, nevertheless it could happen that in dependence from which document the information is extracted we might get multiple possible places. An incomplete database would resolve these contradictions by separating these triples in different possible worlds $W_i \in \mathbf{W}$, where $\mathbf{W}$ is the finite set of all possible worlds. From an incomplete database we do not know which of the worlds in $\mathbf{W}$ is the correct or exact database instance. Probabilistic databases additionally consider a probability distributions over these worlds, where $\sum_{W_i \in \mathbf{W}} P(W_i) = 1$, to differentiate these worlds.

Since an explicit representation of all possible worlds is impractical and can be infeasible if the amount of possible worlds is very large, *probabilistic conditional tables* (pc-tables) are used as a representation system. In this representation system each pc-table represents one relation-type and each tuple t in this table is annotated with a propositional formula $\Phi_t \in \Phi$ over mutually independent random variables X_j, where Φ is the set of all propositional formulas in the database.

Table 7.1: Probabilistic conditional table consisting of the the relation-type `knows` from Figure 7.1a

knows			
Subject	**Object**	**Φ**	**p**
Jack	Jane	X_1	0.7
Jack	Jim	X_2	0.4
Jack	Lucy	X_3	0.3

The set of all values that can be assigned to X_j is defined by its domain, denoted as Dom_{X_j}. Furthermore, the set Θ of all possible assignments to the random variables in Φ is of complexity $\Theta = Dom_{X_1} \times ... \times Dom_{X_j} \times ... \times Dom_{X_m}$ and defines a probability distribution over the assignments of the random variables. Due to the independence assumption, the probability for a specific assignment $\theta \in \Theta$ can be computed by

$$P(\theta) = \prod_{j=1}^{m} P(X_j = b_j) \quad \text{with } b_j \in Dom_{X_j}.$$

From the probabilities of assignments θ we are able to compute the probability for a possible world $W_i \in \mathbf{W}$ by

$$P(W_i) = \sum_{\theta \in \Theta : W^\theta = W_i} P(\theta),$$

meaning that we add up the probabilities of the assignments θ that lead to the associated world W^θ. Computing all possible worlds is in the worst case exponential in the number of random variables in Φ, since we have to try every assignment θ of the set of all possible assignments Θ on the variables in Φ. For the same reason, computing the probability of a single possible world is exponential as well, since we have to compute and add up the probabilities of all valuations on Φ that lead to the possible world W^θ. These kinds of problems are assigned to the complexity class $\#P$ (sharp-P), which includes the set of counting problems associated with the non-polynomial decision problems.

In this work we only consider boolean random variables ($Dom_{X_j} = \{true, false\}$) for triples, because with knowledge graph data triples are either true or false. We further assume triple independence (i.e. *tuple-independent databases*), therefore annotating every ground triple with exactly one boolean random variable. In this case, the database includes exactly n boolean random variables and the set of all possible assignments Θ is of size 2^n, where n is the number of ground triples in the database which is typically in the millions

to billions.

In Table 7.1, an example PDB representation of the `knows` relation-type shown in Figure 7.1a using pc-tables is shown. Each subject/object tuple t is annotated with a propositional formula Φ_t in this table, which in this case is just the random variable X_t that has been assigned to the ground triple. Generally the probability p for a tuple t is derived from the set of satisfying assignments $\omega(\Phi_t)$ of the random variables in the propositional formula Φ_t with

$$P(\Phi_t) = \sum_{\theta \in \omega(\Phi_t)} P(\theta), \tag{7.1}$$

where for ground tuples, the set of satisfying assignments only consists of $X_t = true$, which is the confidence of the e.g. information extractor method used for extracting the triple (relational tuple). For convenience, we have omitted the explicit representation of the counter events, that is a certain triple is believed to be false, denoted by the propositional formula $\neg X_j$. Relational tuples can be annotated with more complex propositional formulas, e.g. after a join of pc-tables. Computing the probability of these formulas can then be reduced to finding all satisfying assignments, which is also exponential in the number of random variables in Φ_t.

The probabilistic database shown in Table 7.1 includes 2^3 possible worlds. The possible world W consisting only of the triple (`Jack`, `knows`, `Jane`) can be only generated by the assignment $\theta = \{X_1 = True, X_2 = false, X_3 = false\}$ and its probability is therefore given by

$$P(W) = P(X_1 = true) \cdot P(X_2 = false) \cdot P(X_3 = false) = 0.7 \cdot 0.6 \cdot 0.7 = 0.294.$$

In the above example, we started from ground triples which have very simple propositional formulas (just one random variable). Pc-tables that arose from manipulations of tables with ground triples, e.g. joins, can lead to very complex propositional formulas for each tuple t represented in the compound pc-table. The complexity of these propositional formulas has great impact on the way queries on these databases can be evaluated, since evaluating queries boils down to evaluating propositional formulas, which is exponential in the number of random variables. Fortunately, it is possible to sometimes avoid exponential algorithm runtimes if certain independence assumptions hold on the query structure. Querying probabilistic databases will be discussed next.

Table 7.2: Probabilistic conditional table consisting of the relation-type `friendOf` from Figure 7.1a

friendOf			
Subject	**Object**	**Φ**	**p**
Jane	Lucy	Y_1	0.4
Jim	Lucy	Y_2	0.8

7.1.3 Querying in Probabilistic Databases

Query evaluation in PDBs remains a major challenge. In particular, scalability to large domains is significantly harder to achieve when compared to deterministic databases.

Of interest here is the *possible answer semantics* which calculates the probability that a given tuple t is a possible answer to a query Q in any world $W \in \mathbf{W}$ of a PDB $\mathbf{D}$. For the marginal probability over all possible worlds, we get

$$P(t \in Q) = \sum_{W \in \mathbf{W}: t \in Q(W)} P(W) \tag{7.2}$$

where $Q(W)$ is the query with respect to one possible world of $\mathbf{D}$. In the previous section, we have discussed that the above formulation is exponential, because computing $P(W)$ for all possible worlds is exponential in the number of random variables present in the set of all propositional formulas Φ and therefore in the number of ground triples in the database $\mathbf{D}$.

An important concept in query evaluation is the lineage expression $\Phi_Q^{\mathbf{D}}$ of a possible answer tuple t to Q with respect to $\mathbf{D}$. The lineage is the propositional formula that represents the event of the output tuple t to a query over the possible worlds $\mathbf{W}$ of $\mathbf{D}$. For example, on the probabilistic database consisting of the collection of pc-tables shown in Table 7.1 and 7.2, the lineage Φ_Q of the query $Q : -\exists y.knows(\texttt{Jack}, y), friendOf(y, \texttt{Lucy})$[3] consists of the propositional formula:

$$\Phi_Q = X_1 Y_1 \vee X_2 Y_2$$

The concept of lineage allows a reduction of the query evaluation problem to the evaluation of propositional formulas. In contrast to the formulation in Equation 7.2, the evaluation of propositional formulas (Equation 7.1) is "only" exponential in the number of random

[3]We ask if Jack knows someone who is a friend of Lucy.

variables included in the propositional formula of the lineage (i.e. the set of ground triples needed for evaluating the query). Further, computing the lineage expression itself for a query $Q(\bar{x})$ with head variables $\bar{x}$ and a possible tuple $\bar{a}$ is polynomial in the set of all constants occurring in the database $\mathbf{D}$ (the active domain) and exponential in the number of variables in the query expression Q [4]. As a conclusion, since the size of the lineage is polynomial in the size of the database and the evaluation of a propositional formula is exponential in the number of included random variables, the evaluation of the lineage expression is also in the worst case exponential in the size of the database.

Fortunately, not all queries necessarily lead to an evaluation that is exponential in the size of $\mathbf{D}$. Often, independence assumption within the query expressions can be exploited that lead to polynomial query evaluations. *Extensional query evaluation* is concerned with queries where the entire probabilistic inference can be computed in a database engine and thus can be processed as effectively as the evaluation of standard SQL queries. This queries are denoted as *safe*. Safe queries can be directly evaluated on query level, without the need to evaluate propositional formulas, except for evaluating the propositional formulas of ground relational tuples, which are each annotated by a single independent boolean random variable.[5] Queries that are not safe are denoted as *unsafe*. These queries can be evaluated by exploiting *intensional query evaluation*, which evaluates the propositional formulas. Every relational query can be evaluated this way, but the data complexity depends dramatically on the query being evaluated, and can be hard for $\#P$.[6] Nevertheless, even though some queries might require intensional query evaluation, extensional query evaluation sometimes might provide a good approximate that suffices for the target application.

For our contribution, we will focus on extensional query evaluation and safe queries, respectively, because they are of major importance for the contributions of this chapter. Intensional query evaluation is not a target of this chapter and we refer to [100], Chapter 5 for details on intensional query evaluation using rules or circuits.

[4] Not to be confused with the number of random variables in $\Phi_{Q(\bar{x})}$.

[5] This also holds for more expressive probabilistic databases, since these databases can be decomposed to tuple-independent databases. [100], Chapter 4

[6] Generally all unsafe queries are in $\#P$ and all safe queries are polynomial. This is known as the dichotomy theorem. Nevertheless, due to the notion of the *sufficient syntactic independence* assumption we might classify certain safe queries as unsafe and perform intensional query evaluation.

Extensional Query Evaluation

Extensional query evaluation only depends on the query expression itself and the lineage does not need to be computed. During the evaluation process, several rules are applied to the query in order to divide it into smaller and easier sub-queries until it reduces to ground tuples with elementary probability values. Queries that can be completely simplified to ground tuples with extensional evaluation rules are *safe*, in the sense mentioned above. This evaluation procedure relies on identifying independent probabilistic events in the query that can be separated, e.g. in case of a join into a conjunction of two simpler queries, where the probabilities of the two sub-queries can simply be multiplied.

It can be decided that two queries are independent probabilistic events if they are *syntactically independent*. *Syntactic independence* of two propositional formulas Φ_{Q_1} and Φ_{Q_2} is given if $Var(\Phi_{Q_1}) \cap Var(\Phi_{Q_2}) = \emptyset$, where $Var(\Phi)$ denotes the set of random variables Φ depends on (known as the *support* of Φ). Unfortunately, the determination of the support of a propositional formula is in general co-NP-complete. In extensional query evaluation it often suffices to exploit a *sufficient condition for syntactic independence* for this purpose which can determine if queries are independent probabilistic events in polynomial time. The sufficient condition syntactic independence is given by $V(\Phi_{Q_1}) \cap V(\Phi_{Q_2}) = \emptyset$, where $V(\Phi)$ denotes the set of random variables that are observed in Φ. Clearly, $Var(\Phi_{Q_1}) \subseteq V(\Phi)$ and therefore propositional formulas that fulfill the sufficient condition for syntactic independence are also syntactically independent (but the converse does not hold). In tuple-independent databases, each ground tuple is associated with a random variable. Therefore two sub-queries Q_1 and Q_2 are guaranteed to be independent probabilistic events if they do not unify, meaning that they share no common tuple.[7] Note that it can be decided if two sub-queries are independent solely based on the query syntax without the need of the lineage expression.

Extensional query evaluation can be implemented via the application of six rules [100], with three of them, especially the independent-project rule, being of major importance for the remaining chapter.

- Independent Join:

$$P(Q_1 \wedge Q_2) = P(Q_1) \cdot P(Q_2) \tag{7.3}$$

[7] Due to the absorption law, there can be syntactically independent queries that unify.

Table 7.3: Probabilistic conditional table consisting of the the relation-type `bornIn`

bornIn			
Subject	**Object**	**Φ**	**p**
Jack	Rome	Z_1	0.4
Jack	London	Z_2	0.5

- Independent Union:

$$P(Q_1 \vee Q_2) = 1 - (1 - P(Q_1)) \cdot (1 - P(Q_2)) \tag{7.4}$$

- Independent-Project:

$$P(\exists x.Q) = 1 - \prod_{a \in ADom} (1 - P(Q[a/x])) \tag{7.5}$$

This rule is applied to queries of the form $\exists x.Q$ if x is a separator variable.[8]

For instance, consider our running example, the probabilistic database consisting of the pc-tables shown in Tables 7.1, 7.2 and additionally Table 7.3. Consider further that we want to know the probability that Jack is born in Rome and that he knows someone who is a friend of Lucy. This query can be written as a conjunction of two sub-queries Q_1 and Q_2,

$$Q_1 \ :- \ \texttt{bornIn}(\texttt{Jack}, \texttt{Rome}) \tag{7.6}$$

$$Q_2 \ :- \ \exists y.(\texttt{knows}(\texttt{Jack}, y), \texttt{friendOf}(y, \texttt{Lucy})) \ . \tag{7.7}$$

Q_1 asks if Jack is born in Rome and Q_2 asks if Jack knows somebody who is a friend of Lucy. By exploiting the independent join rule on Q_1 and Q_2 and the independent-project rule on Q_2, this query can be evaluated as

$$P(Q_1 \wedge Q_2) = P(\texttt{bornIn}(\texttt{Jack}, t)) \times \left(1 - \prod_{a \in ADom} [1 - P(\texttt{knows}(\texttt{Jack}, a)) \cdot P((\texttt{friendOf}(a, \texttt{Lucy}))]\right) . \tag{7.8}$$

[8] x is a separator variable if it occurs in all relational atoms in Q and if in the case that atoms unify, x occurs at a common position.

Note that a person can know many other persons and therefore the `knows` relations in Q_2 are not mutually exclusive. This induces a complex expression that is not simply the sum or the product of probabilities.

7.2 Exploiting Latent Variable Models for Querying

As discussed in the introduction for this chapter, we can exploit latent variable models for learning a probability distribution over all possible triples (with considering type-constraints) of the knowledge graph. This probability distribution can be exploited for constructing a probabilistic database. The naive approach for realizing probabilistic querying on this database would be to infer all probabilities from the latent variable model and save them in the database together with the corresponding triples. Then, we could query this database as any other probabilistic database, exploiting extensional and intensional query evaluation algorithms.

Obviously, this approach is intractable for larger knowledge graphs, because the amount of possible triples is simply too large. The Freebase sample shown in Table 4.2 contains already 57 billion possible triples and saving these triples together with the probabilities would consume approximately 1TB of storage[9]. Note that this sample is considerably small compared to whole Freebase, e.g. it contains only 0.3% of the Topic entities and 0.4% of the relation-types of Freebase (see Chapter 2.3.2).

As an alternative, we could compute the probabilities "on demand" for those triples that are of interest for the current query or sub-query and apply the query evaluation rules afterwards. This approach would avoid storage explosion, but introduces additional computational load on the query evaluation, which can be tremendous. Note that no matter if the query is safe or unsafe we would have to compute $|Var(\Phi_Q)|$ probabilities, which is the number of random variables (i.e. ground triples) the query depends on. Below, we exemplify this issue based on a series of simple safe queries.

Consider the relational tuple $\texttt{knows}(\texttt{Jane}, \texttt{Jim})$. The probability of this relation is computed from a latent variable model θ (any of the methods described in Chapter 3.3) by

$$P(\texttt{knows}(\texttt{Jane}, \texttt{Jim})) = \psi(\theta_{\texttt{Jane,knows,Jim}}),$$

where $\theta_{s,p,o}$ denotes the confidence of the latent variable model into the relation that Jane

[9]Considering that each triple is saved by 32 bit integer values and the probability by one 32 bit float value.

knows Jim and $\psi(x) \in (0, 1]$ maps this confidence value to a valid probability space through e.g. Platt Scaling (see Equation 6.2 or [87]).

If we need to know the probability that anybody knows Jim ($Q :- \exists y.\texttt{knows}(y, \texttt{Jim})$ we would have to compute $|ADom|$ evaluations of the latent variable model. If we further assume the query

$$Q :- \exists y.\texttt{knows}(\texttt{Jack}, y), \texttt{friendOf}(y, \texttt{Lucy}),$$

which is evaluated by applying the independent-project rule as

$$P(Q) = \left(1 - \prod_{a \in ADom} [1 - P(\texttt{knows}(\texttt{Jack}, a)) \cdot P((\texttt{friendOf}(a, \texttt{Lucy}))]\right),$$

we can observe that it needs $2 \times |ADom|$ evaluations of the latent variable model. In many cases it can also be of interest to extract a ranking over all persons in the database that are a friend of `Lucy` with

$$Q(x) :- \exists y.\texttt{knows}(x, y), \texttt{friendOf}(y, \texttt{Lucy}),$$

to get the persons that most likely know friends of the entity. For his query we would need $2 \times |ADom|^2$ evaluations of the latent variable model. The structure of the above query can even lead to cubic evaluations in $|ADom|$ of the model, if we modify the query to

$$Q(x) :- \exists y.(\texttt{knows}(x, y), \exists z.\texttt{friendOf}(y, z)),$$

where we introduced another existential quantifier for the second variable in the relation-type `friendOf` by querying for all persons that know someone who has friends. This query is evaluated as

$$P(Q(x)) = \left(1 - \prod_{a_1 \in ADom} [1 - P(\texttt{knows}(x, a_1)) \cdot \left(1 - \prod_{a_2 \in ADom} [1 - P(\texttt{friendOf}(a_1, a_2))\right)\right)$$

The complexity is mainly caused by nested computations introduced by the existentially quantified query variables and their product-aggregation in the independent-project rule (Equation (7.5)).

It is expected that the computation of the probabilities from the latent variable models will have significant negative impact on the total query evaluation time, especially when evaluating with the independent-project rule.

The key idea is to reduce the amount of evaluations of latent variable models through approximating safe sub-queries of the type $\exists x.Q$ by exploiting intrinsic features of latent variable models. Through this approach, we avoid costly evaluations of sub-queries and additionally construct materialized views that have a memory efficient latent representation. To illustrate the proposed approach, consider the queries Q_1 and Q_2 from Equations 7.6 and 7.7. Q_1 does not include any existential quantifier and therefore we simply compute the probability value from the model. In Q_2, an existential quantifier for the variable y is present. As discussed before, the calculation of queries that have a similar structure as Q_2 can become very expensive. To overcome this problem, we approximate the probabilistic answer to Q_2 by a two-step process. First, we create a newly formed compound relation `knowsFriendOf`, which represents the database view generated by Q_2,

$$Q_2(x, z) : -\texttt{knowsFriendOf}(x, z).$$

To create the compound relation, we use the deterministic and sparse representation of the affected relations from Q_2 and join them into a single relation. This avoids the expensive calculation of probabilities for each instance of the active domain of y and can be computed efficiently, as the deterministic join is not expensive, if the (deterministic) domain is sparse. However, the representation of Q_2 would only be based on the available deterministic information so far and would not utilize the probabilistic model of the knowledge graph computed by the latent variable model. Hence, in a second step we now need to derive probabilities for the triples in the newly formed compound relation. Fortunately, all that is needed to derive these probabilities under a latent variable model such as RESCAL or TransE is to compute a latent representation of the newly created compound relation `knowsFriendOf`, which can be done very efficiently.[10] Depending on the latent variable model, the procedure for learning the latent representation of the compound relation differs. In the next subsection we will describe how a new compound relation can be learned with RESCAL, TransE and the multiway neural network approach exploited in the Google Knowledge Vault project (mwNN).

[10]Note that it is assumed for the new compound relation that all triples are independent and for this reason it can be exploited as view. Generally, extensional query evaluation exploits the possible answers semantics which is not compositional, meaning that the computed probabilities do not represent a probabilistic database, but a collection of probabilities that cannot be exploited for further querying.

7.2.1 Learning Compound Relations with RESCAL

Let $\hat{\mathbf{X}}_{(*)}$ denote the newly created type-constrained compound relation and $\mathbf{domain}_{(*)}$ and $\mathbf{range}_{(*)}$ its domain and range, which can be easily derived from the joined relation-types. Furthermore, assume that a meaningful latent representation of the entities has been explored via the factorization of the deterministic triple store. Since the RESCAL model uses a unique representation of entities over all relations, all that is needed to derive probabilities for a new relation is to compute its latent representation $\mathbf{R}_{(*)}$. The big advantage of the proposed method is that $\mathbf{R}_{(*)}$ can now be derived by simply projecting $\hat{\mathbf{X}}_{(*)}$ into the latent space that is spanned by the type-constrained embedding matrices of entities $\mathbf{A}_{[\mathbf{domain}_{(*)},:]}$ and $\mathbf{A}_{[\mathbf{range}_{(*)},:]}$. This can be done very efficiently. Consider the type-constrained ALS update for the core tensor $\underline{\mathbf{R}}$ from Chapter 5.1.2. Essentially, what is necessary is to calculate the latent matrix for the materialized view, i.e., $\mathbf{R}_{(*)}$ as

$$\begin{aligned} \mathbf{R}_{(*)} \quad &= \quad ((\mathbf{C} \otimes \mathbf{B})^T(\mathbf{C} \otimes \mathbf{B}) + \lambda \mathbf{I})^{-1}(\mathbf{C} \otimes \mathbf{B})^T vec(\hat{\mathbf{X}}_k) \\ &with \quad \mathbf{B} = \mathbf{A}_{[\mathbf{domain}_{(*)},:]} \; and \; \mathbf{C} = \mathbf{A}_{[\mathbf{range}_{(*)},:]}. \end{aligned} \tag{7.9}$$

It was shown in Chapter 5.1.2 that this closed-form solution can be calculated more efficiently by exploiting the singular value decomposition of the type-constrained factor matrices $\mathbf{A}_{[\mathbf{domain}_{(*)},:]} = \mathbf{U}_\mathbf{B}\mathbf{\Sigma}_\mathbf{B}\mathbf{V}_\mathbf{B}^T$ and $\mathbf{A}_{[\mathbf{range}_{(*)},:]} = \mathbf{U}_\mathbf{C}\mathbf{\Sigma}_\mathbf{C}\mathbf{V}_\mathbf{C}^T$, leading to

$$\mathbf{R}_{(*)} = \mathbf{V}_\mathbf{B}(\mathbf{P} \circledast \mathbf{U}_\mathbf{B}^T\hat{\mathbf{X}}_{(*)}\mathbf{U}_\mathbf{C})\mathbf{V}_\mathbf{C}^T \tag{7.10}$$

where $\circledast$ represents the Hadamard (element-wise) matrix product and $\mathbf{P}$ has been defined as follows (Chapter 5.1.2): Let $\mathbf{Q}$ be defined as a diagonal matrix and its diagonal entry q_{ii} be given by

$$\begin{aligned} q_{ii} \quad &= \quad \frac{\mathbf{D}_{\mathbf{B}_{ii}}\mathbf{D}_{\mathbf{C}_{ii}}}{\mathbf{D}_{\mathbf{B}_{ii}}^2\mathbf{D}_{\mathbf{C}_{ii}}^2 + \lambda} \\ \text{with } \mathbf{D}_\mathbf{B} \quad &= \quad \Sigma_\mathbf{B} \otimes \Sigma_\mathbf{B} \text{ and } \mathbf{D}_\mathbf{C} = \Sigma_\mathbf{C} \otimes \Sigma_\mathbf{C}. \end{aligned}$$

Then $\mathbf{P}$ can be constructed by a column-wise reshape of the diagonal in $\mathbf{Q}$.

The calculation of the latent representation $\mathbf{R}_{(*)}$ for the newly created compound relation-type can now be done in $\mathcal{O}(r^3 + n_{(*)}r + m_{(*)}r + pr)$, where p represents the number of nonzero entries in $\hat{\mathbf{X}}_{(*)}$, r represents the rank of the factorization, and where $n_{(*)}$ represents all entities in the domain and $m_{(*)}$ represents all entities in the range of the

compound relation-type $(*)$. Please note that the computation of $\mathbf{R}_{(*)}$ is now *linear* in all parameters regarding the size of the triple store and cubic only in the number of latent components r that are used to factorize the triple store. As such, it can be computed efficiently even for very large triple stores. Furthermore, for each query of the same type, the same latent representation can be reused, i.e. $\mathbf{R}_{(*)}$ only needs to be computed once.

7.2.2 Learning Compound Relations with TransE and mwNN

Similar to RESCAL, we are also able to learn new latent representations for compound relation-types with TransE and mwNN, but in contrast to RESCAL we are not able to exploit a closed-form solution for this. Let again $\hat{\mathbf{X}}_{(*)}$ denote the newly created compound relation with type-constraints $\mathbf{domain}_{(*)}$ and $\mathbf{range}_{(*)}$, which have been derived from the joined relation-types. We also assume that the latent representations for the entities have been inferred from a sufficient amount of data such that they are stable. In other words, we assume that we have already found good representations for entities. Further, in case of the neural network model, we also assume that the network weights have reached a stable local minimum. We then learn the new representation of the compound relation-type through stochastic gradient descent considering all model parameters as constant except for the new latent representation $\mathbf{r}_{(*)}$. Below, we will provide the update rules for both models, TransE and mwNN, for learning $\mathbf{r}_{(*)}$.

Updating $\mathbf{r}_{(*)}$ with TransE

For each triple $(s,(*),o)$ drawn from the compound relation $(*)$, the loss function of TransE is given as

$$\begin{aligned} \mathcal{L}^{\mathcal{TC}(*)}_{TransE} &= \mathbf{max}\{0, \gamma + \theta_{s',(*),o} - \theta_{s,(*),o}\} + \mathbf{max}\{0, \gamma + \theta_{s,(*),o'} - \theta_{s,(*),o}\} \quad (7.11) \\ \text{where} \quad & s' \in \mathcal{E}_{[\mathbf{domain}_{(*)}]} \subseteq \mathcal{E},\ o' \in \mathcal{E}_{[\mathbf{range}_{(*)}]} \subseteq \mathcal{E}, \\ \text{and where for} \quad & \text{any triple } (s,p,o),\ \theta_{s,p,o} = -\delta(\mathbf{a}_s + \mathbf{r}_p, \mathbf{a}_o). \end{aligned}$$

We update the latent representation $\mathbf{r}_{(*)}$ of the compound relation $\hat{\mathbf{X}}_{(*)}$ with respect to the triple $(s,(*),o)$ as

$$\mathbf{r}_{(*),t+1} = \mathbf{r}_{(*),t} - \alpha \frac{\partial \mathcal{L}_{TransE}^{\mathcal{TC}(*)}}{\partial \mathbf{r}_{(*),t}} \tag{7.12}$$

with

$$\frac{\partial \mathcal{L}_{TransE}^{\mathcal{TC}(*)}}{\partial \mathbf{r}_{(*),t}} = \begin{cases} 0 & \textbf{if } \theta_{s,(*),o} - \theta_{s',(*),o} \leq \gamma \wedge \theta_{s,(*),o} - \theta_{s,(*),o'} \leq \gamma \\ 2\mathbf{a}_{o'} - 2\mathbf{a}_o & \textbf{if } \theta_{s,(*),o} - \theta_{s',(*),o} \leq \gamma \\ 2\mathbf{a}_s - 2\mathbf{a}_{s'} & \textbf{if } \theta_{s,(*),o} - \theta_{s,(*),o'} \leq \gamma \\ 2\mathbf{a}_{o'} - 2\mathbf{a}_o + 2\mathbf{a}_s - 2\mathbf{a}_{s'} & \textbf{else}. \end{cases}$$

In the above update, the index t denotes the learned latent representation $\mathbf{r}_{(*)}$ after t updates. Further, α denotes the learning rate.

Updating $\mathbf{r}_{(*)}$ with mwNN

For each triple $(s,(*),o)$ drawn from the compound relation $(*)$, the loss function of mwNN is given as

$$\mathcal{L}_{mwNN}^{\mathcal{TC}(*)} = -\log \theta_{s,(*),o} - \sum_{o' \in \mathcal{E}_{[\mathbf{range}_{(*)}]} \subseteq \mathcal{E}}^{c} \log(1 - \theta_{s,(*),o'}) \tag{7.13}$$

$$\text{where for any triple } (s,p,o),\ \theta_{s,p,o} = \sigma(\beta^T \phi(\mathbf{W}[\mathbf{a}_s, \mathbf{r}_p, \mathbf{a}_o])).$$

We update the latent representation $\mathbf{r}_{(*)}$ of the compound relation $\hat{\mathbf{X}}_{(*)}$ with respect to the triple $(s,(*),o)$ as

$$\mathbf{r}_{(*),t+1} = \mathbf{r}_{(*),t} - \frac{\alpha}{\sqrt{\sum_{t'=1}^{t} \left(\frac{\partial \mathcal{L}_{mwNN,t'}^{\mathcal{TC}(*)}}{\partial \mathbf{r}_{(*),t'}} \right)^2}} \cdot \frac{\partial \mathcal{L}_{mwNN}^{\mathcal{TC}(*)}}{\partial \mathbf{r}_{(*),t}} \tag{7.14}$$

with

$$\frac{\partial \mathcal{L}_{mwNN}^{\mathcal{TC}(*)}}{\partial \mathbf{r}_{(*),t}} = -\frac{1}{\theta_{s,(*),o}} \cdot \frac{\partial \theta_{s,(*),o}}{\partial \mathbf{r}_{(*),t}} - \sum_{o' \in \mathcal{E}_{[\mathbf{range}_{(*)}]} \subseteq \mathcal{E}}^{c} \frac{1}{1 - \theta_{s,(*),o'}} \cdot -\frac{\partial \theta_{s,(*),o'}}{\partial \mathbf{r}_{(*),t}}$$

$$\text{where for any triple } (s,p,o)$$

$$\frac{\partial \theta_{s,p,o}}{\partial \mathbf{r}_p} = \theta_{s,p,o}(1 - \theta_{s,p,o})\beta^T \left(\left[1 - \phi(\mathbf{W}[\mathbf{a}_s, \mathbf{r}_p, \mathbf{a}_o])^2 \right] \bullet \mathbf{W}_{\mathbf{r}} \right)$$

Again, the index t denotes the learned latent representation $\mathbf{r}_{(*)}$ after t updates and in Equation 7.14 the fraction incorporating the learning rate α describes the adaptive learning rate [26]. $\mathbf{W}_\mathbf{r}$ denotes only that part of the weight matrix $\mathbf{W}$ that interacts with the latent representations of relation-types in the matrix product $\mathbf{W}\,[\mathbf{a}_s, \mathbf{r}_p, \mathbf{a}_o]$. $\bullet$ denotes the column-wise product between a vector and a matrix.

7.2.3 Numerical Advantage of Learned Compound Relation-Types

In addition to the decrease in evaluations of the latent variable model to generate the required probabilities there is also a numerical advantage of the learned compound relation regarding its probabilities. Consider the query

$$Q(x) : -\exists y.\texttt{knows}(x, y), \texttt{friendOf}(y, \texttt{Lucy}),$$

which can be evaluated with the independent-project rule as

$$P(Q(x)) = \left(1 - \prod_{a \in ADom} [1 - P(\texttt{knows}(x, a)) \cdot P((\texttt{friendOf}(a, \texttt{Lucy}))]\right).$$

For relation-types with a large domain or range, the above product can range over thousands of different values of a, namely all entities that are in common by the range of the first relation-type (in the above example `knows`) and the domain of the second relation-type (`friendOf` in the above example). As a consequence, the product of all probabilities $\prod_{a \in ADom}[1 - P(\texttt{knows}(x, a)) \cdot P((\texttt{friendOf}(a, \texttt{Lucy}))]$ will quickly evolve beyond machine precision. As a simple example, assume that the above product loops over 10,000 entities. It makes no difference if the probabilities $1 - P(\texttt{knows}(x, a)) \cdot P((\texttt{friendOf}(a, \texttt{Lucy}))$ are all 0.99 or 0.01. The probability for the query $P(Q(x))$ will be exactly 1.0 for any x. Obviously, ranking the results is pointless in this case. Note that due to the structure of the independent-project rule, substituting the product of probabilities through the sum of logarithmic probabilities,

$$P(Q) = 1 - \exp(\sum_{a \in ADom} \log(1 - P(\texttt{knows}(\texttt{Jack}, a)) \cdot P((\texttt{friendOf}(a, \texttt{Lucy})))),$$

does not provide a solution for this problem because the exponent will be a very large negative value.

The learned compound relation-types on the other hand will contain probabilities that

Table 7.4: Data sets used in the experiments.

Data Set	Entities	Relation-Types	Triples
Nations	14	56	2,565
UMLS	135	49	6,752
DBpedia-Music	71,804	7	508,169

have an order, because they will not exceed machine precision. Furthermore, in case $P(Q(x))$ is a sub-query, the learned compound relation will influence the probability of the whole query, which is not the case for the probabilities of the compound relation-type derived by extensional query rules. These are very likely to be exactly 1.

7.3 Evaluating the Learned Compound Relations

First, we will study the quality of the learned compound relation-types in general, before turning to actual probabilistic querying of statistically modeled knowledge graphs. For this reason we conducted experiments on various smaller and simple benchmark data sets, namely the Nations and UMLS data sets [11]. With these data sets, we are able to materialize all compound relations and will also not run into numerical problems (Section 7.2.3). Therefore, we can easily study the quality of the learned compound relation-type. We do this by comparing the ranking of the probabilities in the compound relation-types that have been constructed through extensional query evaluation or through learning as described in the previous section. Furthermore, we are exploiting the RESCAL tensor factorization method in the experiments, due to its superior fast training times.[12]

7.3.1 Experimental Setup

For both data sets, Nations and UMLS (Table 7.4), we followed the same procedure. We started by searching for the best hyper-parameters based on 80% of the triples through 10-fold cross-validation and used the best parameter setting to retrain the model on the complete data sets. From the resulting factorization, we constructed all possible compound relations of the form $\exists y.L_i(x,y), L_j(y,z)$ in two different ways. First, we exploit extensional query evaluation and even though the resulting compound relation is not a view, it still

[11] http://alchemy.cs.washington.edu/data/

[12] In addition, due to the results from Chapter 5.4 it can be expected that the results of TransE or mwNN will be at least of similar quality as the results obtained through RESCAL.

represents valid probabilities of each triple in the compound relation. Second, we learn the compound relation-types as views as described in Section 7.2.1 (Equation 7.10).

For the comparison of both approaches, we assume that the extensional query evaluation results in a correct ranking of probabilities in the compound relation-type (our gold standard). For this reason we binarize the compound relation-type derived through extensional query evaluation, where the top k triples with the highest probability are assumed true (or one) and the other are assumed as false (or zero). We define k as the number of true triples in the deterministic compound relation between the deterministic versions of the relation-types L_i and L_j. We then compare the ranking of triples in the learned compound relation to the above defined gold standard derived from the extensional query evaluation in terms of the Area Under the Precision Recall Curve (AUPRC). In addition, we also report the results when comparing the gold standard against a random ranking. For each compound relation we repeated the comparison against random ten times and used the median as final score.

We report the median[13] and standard deviation of the AUPRC scores on all possible compound relation-types (without self joins), where we only considered compound relations that contained more than 10 triples.

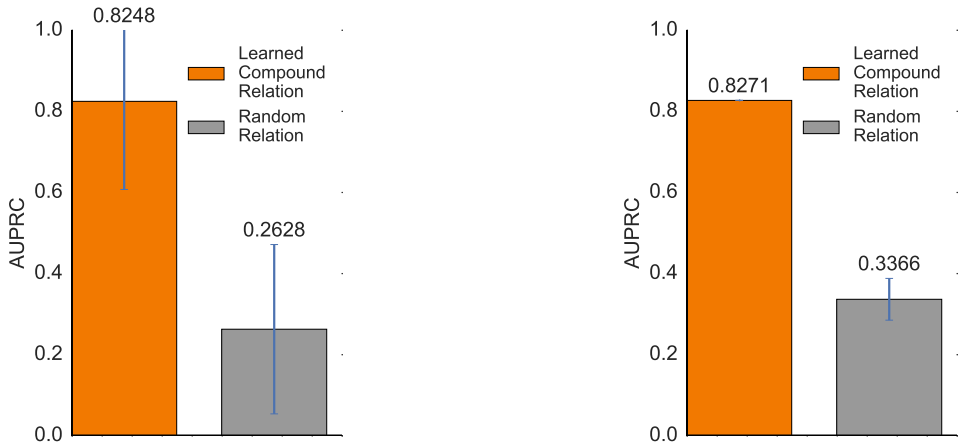
7.3.2 Compound Relations are of Good Quality

In Figures 7.2 and 7.3 the results for the Nations and UMLS data sets are shown. Generally, the compound relation-types learned from the deterministic compound relation-type result in a very similar ranking as the compound relation-type obtained by the extensional query evaluation rules, which served as gold standard.

In case of the Nations data set, 2,354 compound relations were evaluated. The ranking in the learned compound relation-type agrees with the ranking of the gold standard with a median AUPRC score of 0.8248 and for 83 compound relation-types the AUPRC score is above 0.99 (standard deviation is 0.2174). The ranking of a random relation-type on the other hand results in clearly less agreement with the gold standard (grey bar), as expected.

For the UMLS data set, 631 compound relation-types were evaluated. In this case, we have strong agreement between both kinds of compound relation-types, the learned compound relation and the one derived through extensional query evaluation. The median AUPRC score is almost perfect (0.9970) and clearly differs from the agreement achieved by a random relation-type (AUPRC:0.0034).

[13]We report the median because of its robustness to outliers.



(a) Results based on all 2354 compound relations

(b) *negativeBehaviorToAlliedNationOf*

Figure 7.2: AUPRC results on the Nations data set. We compare the ranking of triples in the compound relations learned from the deterministic compound relation to the gold standard (orange bars); the gold standard is the compound relation derived through extensional query evaluation rules. The AUPRC score for random compound relations is shown in grey. (a) Median AUPRC scores of all 2,354 computed compound relations. (b) AUPRC score for a single compound relation ($negativeBehaviorToAlliedNationOf$)

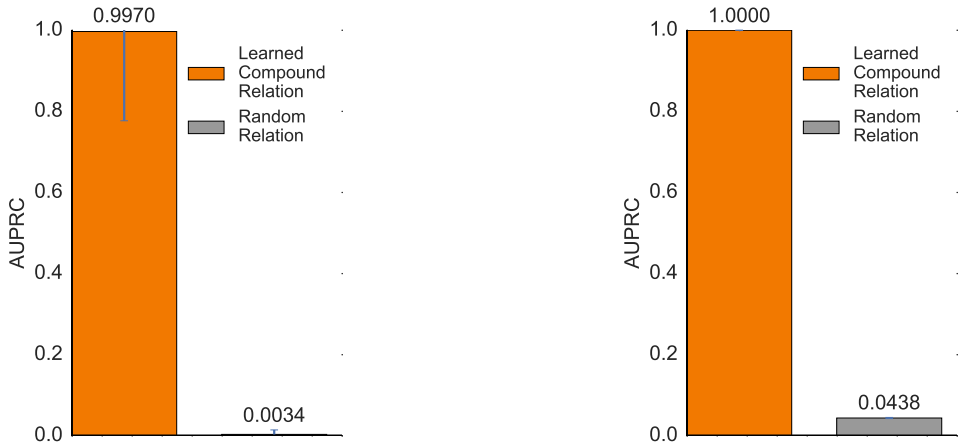
From the results it can be inferred that the approximation of the compound relation-types by learning the deterministic compound relation-type is very promising to be applied in a query evaluation setting on knowledge graphs, which we will study next.

7.4 Querying Factorized DBpedia-Music

In this section, we study the application of latent variable models for querying knowledge graphs with uncertainties. We further compare the two approaches discussed before, namely approximating sub-queries by learning compound relations with the latent variable model and by evaluating solely based on extensional query evaluation rules. For the knowledge graph, we extracted relation-types, entities and type-constraints from the music domain of DBpedia [66] and exploited RESCAL as latent variable model.

7.4.1 DBpedia-Music

DBpedia contains the structured information extracted from Wikipedia Infoboxes. For the DBpedia-Music data set, we downloaded the owl-ontology, mapping-based-properties



(a) Results based on all 631 compound relations

(b) *associatedAndResultOf*

Figure 7.3: AUPRC results on the UMLS data set. We compare the ranking of triples in the compound relations learned from the deterministic compound relation to the gold standard (orange bars); the gold standard is the compound relation derived through extensional query evaluation rules. The AUPRC score for random compound relations is shown in grey. (a) Median AUPRC scores of all 631 computed compound relations. (b) AUPRC score for a single compound relation ($associatedAndResultOf$)

(cleaned), mapping-based-types and heuristics from the canonicalized data sets of the current release of DBpedia[14]. We extracted triples from 7 pre-selected Object-Properties; `musicalBand`, `musicalArtist`, `associatedMusicalArtist`, `recordLabel`, `album`, `genre`, `associatedBand`, where `genre` has been extracted to include only those entities that were covered by the other object-properties to restrict it to musical genres. We discarded all triples of entities that occurred less than five times and for all of the remaining entities that are not assigned to any class we assigned them to `owl#Thing`. The `rdfs:domain` and `rdfs:range` concepts for the above relation-types were extracted from the DBpedia ontology, where we defined the domain or range of a relation-type as `owl#Thing` if absent. The triples that disagreed with the domain and range constraints of the corresponding relation-type were added to the type-constraints of that relation-type.

7.4.2 Experimental Setup

We split the data set into a test and training set, where 20% of the triples are contained in the test set and 80% in the training set. For hyper-parameter tuning we performed 10-fold

[14]http://wiki.dbpedia.org/Downloads2014

cross-validation on the training set. The final model is trained on the complete training set with the best hyper-parameters. We exploit this model for evaluating the various queries on the DBpedia-Music data set in two ways:

1. We evaluate the queries solely based on extensional query evaluation rules, using the probabilities generated by the trained model.

2. We evaluate the same queries based on extensional query evaluation rules, but with additionally approximating suitable sub-queries by learning the compound relation-type from the deterministic version of the compound relation with the latent variable model (RESCAL).

The quality of the answers (the ranking of probabilities) generated by the two query evaluation approaches is evaluated against three ground truths:

1. The deterministic answers of the database consisting of the training set. We evaluate the inference of known answers.

2. The deterministic answers which were not included in the training set (answers of (test set $\cup$ training set) $\setminus$ answers of training set). We evaluate the inference of new answers.

3. The deterministic answers of the database consisting of the whole data sets (answers of (test set $\cup$ training set)). We evaluate the total inference quality.

We measure the AUPRC, AUROC and the Logarithmic Loss. The Logarithmic Loss,

$$logloss = -\frac{1}{N}\sum_{i=1}^{N}\left(y_i \log(p_i) + (1-y_i)\log(1-p_i)\right),$$

is widely used to evaluate the quality of the probabilities generated by statistical models, whereas in difference to the AUPRC and AUROC a better performance is indicated by a lower value.

We further compare the computation time when evaluating the queries purely rule based with the evaluation procedure where we exploit extensional rules and approximate sub-queries through compound relations learned by the model. All models are implemented in python and the runtime measurements were taken with an Intel(R) Xeon(R) CPU E7-4850 v2. We factorized the knowledge graph data with RESCAL using a rank of 200.

7.4.3 Queries Used for Evaluation

We will now describe the various queries used for the experiments and also give details to their computation.

1. What songs or albums from the Pop-Rock genre are from musical artists that have/had a contract with Atlantic Records?

   $$Q_1(x) : -\texttt{genre}(x, \mathsf{Pop\_rock}) \wedge \exists y.(\texttt{musicalArtist}(x, y) \wedge \texttt{recordLabel}(y, \mathsf{Atlantic\_Records})).$$

   This query is evaluated by extensional query evaluation rules as

   $$Q_1(x) = P(\texttt{genre}(x, z)) \times \left[1 - \prod_{b \in ADom} 1 - P(\texttt{musicalArtist}(x, b) \cdot P(\texttt{recordLabel}(b, \mathsf{Atlantic\_Records}))\right].$$

   and by exploiting the learned compound relation `songsAndAlbumsFromRecordLabel` learned from compound relation consisting of the relation-types `musicalArtist` and `recordLabel` as

   $$Q_1(x) = P(\texttt{genre}(x, \mathsf{PopRock})) \times P(\texttt{songsAndAlbumsFromRecorLabel}(x, \mathsf{Atlantic\_Records}))\ ,$$

2. Which musical artists from the Hip Hop music genre were involved in a single that was produced by Shady (SD), Aftermath (AM) or Death Row (DR) records?

   $$Q_2(x) : -\exists y.(\texttt{genre}(x, \{\mathsf{Hip\_hop\_music}, \mathsf{Hip\_hop}\}) \wedge \texttt{musicalArtist}(y, x) \wedge \texttt{recordLabel}(y, \{\mathsf{SD}, \mathsf{AM}, \mathsf{DR}\}))$$

This query is evaluated by extensional query evaluation rules as

$$Q_2(x) = \left[1 - \prod_{a \in \{\mathsf{Hip\_hop\_music}, \mathsf{Hip\_hop}\}} 1 - P(\texttt{genre}(x, a))\right] \times \left[1 - \prod_{b \in ADom} 1 - P(\texttt{musicalArtist}(b, x) \left[1 - \prod_{c \in \{\mathsf{SD}, \mathsf{AM}, \mathsf{DR}\}} 1 - P(\texttt{recordLabel}(b, c))\right]\right].$$

and by exploiting the learned compound relation `musicalArtistWithSongsByRecordLabel` learned from compound relation consisting of the transpose of the relation-type `musicalArtist` and relation-type `recordLabel` as

$$Q_2(x) = \left[1 - \prod_{a \in \{\mathsf{Hip\_hop\_music}, \mathsf{Hip\_hop}\}} 1 - P(\texttt{genre}(x, a))\right] \times \left[1 - \prod_{c \in \{\mathsf{SD}, \mathsf{AM}, \mathsf{DR}\}} 1 - P(\texttt{musicalArtistWithSongsByRecordLabel}(x, c))\right].$$

3. Which musical artists from the Hip Hop music genre are associated with musical artists that have/had a contract with Interscope Records and are involved in an album whose first letter is a "T"?

$$Q_3(x) : -genre(x, \mathsf{Hip\_hop\_music}) \wedge \exists y.(associatedMusicalArtist(x, y) \wedge \texttt{recordLabel}(y, \mathsf{Interscope\_Records})) \wedge \exists z.\exists t.(\texttt{musicalArtist}(z, x) \wedge \texttt{album}(z, \{\mathsf{Album\ T.*}\}))$$

This query is evaluated by extensional query evaluation rules as

$$Q_3(x) = \left[1 - \prod_{a \in \{\mathsf{Hip\_hop\_music}, \mathsf{Hip\_hop}\}} 1 - P(\texttt{genre}(x, a))\right] \times$$
$$\left[1 - \prod_{b \in ADom} 1 - P(\texttt{assocMusicalArtist}(x, b) \cdot P(\texttt{recLabel}(b, \mathsf{Interscope\_Records}))\right] \times$$
$$\left[1 - \prod_{c \in ADom} 1 - P(\texttt{musicalArtist}(c, x)\left[1 - \prod_{d \in \{\mathsf{Album\ T.*}\}} 1 - P(\texttt{album}(c, d))\right]\right].$$

and by exploiting the learned compound relations `associatedMusicalArtistFromRecordLabel`, learned from compound relation consisting of the relation-types `associatedMusicalArtist` and `recordLabel`, and `musicalArtistFromAlbum`, learned from compound relation consisting of the relation-types `musicalArtist` and `album`, as

$$Q_3(x) = \left[1 - \prod_{a \in \{\mathsf{Hip\_hop\_music}, \mathsf{Hip\_hop}\}} 1 - P(\texttt{genre}(x, a))\right] \times$$
$$P(\texttt{associatedMusicalArtistFromRecordLabel}(x, \mathsf{Interscope\_Records})) \times$$
$$\left[1 - \prod_{d \in \{\mathsf{Album\ T.*}\}} 1 - P(\texttt{musicalArtistFromAlbum}(x, d))\right].$$

7.4.4 Learned Compound Relations Improve Quality of Answers

The results for the queries $Q_1(x)$, $Q_2(x)$ and $Q_3(x)$ are shown in Table 7.5, 7.6 and 7.8, respectively. In general, the generated answers of both evaluation approaches that exploit the probabilities generated by the latent variable models ("Extensional" and "Learned" in the Tables) are always clearly better than random answers ("Random" in the Tables), independent from the query or the ground truth the answers are evaluated against.

When comparing the two approaches, the approach that exploits the compound relations learned from the deterministic compound relations results generally in better probabilities for the answer. This conclusion can be drawn from the fact that the LogLoss score of this query evaluation approach is always significantly better (LogLoss scores of "Learned" in the Tables. Lower values are better.). In case of the AUPRC and AUROC

scores, it depends on the query and corresponding ground truth the answers are evaluated against.

Evaluation of Query $Q_1(x)$

Table 7.5: AUPRC, AUROC and LogLoss scores for evaluating $Q_1(x)$ on DBpedia-Music: *What songs or albums from the Pop-Rock genre are from musical artists that have/had a contract with Atlantic Records?*. Compared are three different evaluation procedures for the query. **Extensional** denotes the evaluation based on pure extensional query evaluation, where RESCAL is used to generate the probabilities. **Learned** additionally approximates sub-queries to avoid evaluations through the independent-project rule. **Random** denotes a ranking of random probabilities. We further compare the answers of these methods against three different set of answers which are described in the column **Ground Truth**.

Evaluating $Q_1(x)$ (RESCAL)

Ground Truth	Evaluated with	AUPRC	AUROC	LogLoss
Known Answers *(Training set)*	**Extensional** *query rules only*	0.4738	0.9620	0.6708
	Learned *compound relation*	**0.6338**	**0.9915**	**0.0993**
	Random *answer*	0.0038	0.5	0.9986
All Answers *(Test set ∪ Training set)*	**Extensional** *query rules only*	0.3849	0.9042	0.6563
	Learned *compound relation*	**0.5714**	**0.9503**	**0.0934**
	Random *answer*	0.0072	0.5	0.9968
New Answers *(All Answers \ Known Answers)*	**Extensional** *query rules only*	**0.2484**	0.8390	0.6931
	Learned *compound relation*	0.1893	**0.9027**	**0.1237**
	Random *answer*	0.0032	0.5	1.0038

The evaluation results of query $Q_1(x)$, *What songs or albums from the Pop-Rock genre are from musical artists that have/had a contract with Atlantic Records?*, are shown in Table 7.5. Regarding the ground truths, the amount of ("Known Answers") is 71 out of 19,257 possible answers. In addition, there are 66 new answers produced if the test set is added to the deterministic database. When comparing the query evaluation that exploits pure extensional query evaluation ("Extensional") with the evaluation approach that additionally approximates sub-queries through learned compound relation-types ("Learned"), three important observations can be made. First, the latter approach is better in retrieving *known answers* which the deterministic database consisting of the training set would produce (AUPRC of 0.6338 vs. 0.4738). The former on the other hand seems to result in a better ranking of *new answers* that could only be given by the database comprising the whole data set (training and test set), where it reaches an AUPRC of 0.2484 compared to

0.1893 of the other approach.

Second, from the AUROC scores we can infer that the approach that exploits the learned compound relations has a slightly better recall than the approach that relies solely on extensional query evaluation. For the known answers it achieves an AUROC of 0.9915 and for new answers 0.9027, whereas the "Extensional" evaluation reaches only 0.9620 and 0.8390.

Third, as mentioned early, both evaluation approaches differ significantly in their LogLoss scores. The evaluation with learned compound relation clearly outperforms the other method with a logloss score of 0.0993 for known answers and 0.1237 for new answers, whereas pure extensional query evaluation is 0.6708 and 0.6931. This has a significant impact on the interpretation of the AUPRC score. We can conclude that even though the evaluation with learned compound relations results in a worse ranking, the resulting probabilities are much more meaningful. Meaningful probabilities allow us to easily filter the answers generated by the evaluation approach, discarding answers with lower probability. In other words, we can directly determine if an answer is likely to be wrong.

Evaluation of Query $Q_2(x)$

The evaluation results of query $Q_2(x)$, *Which musical artists from the Hip Hop music genre involved in a single that was produced by Shady, Aftermath or Death Row records?*, are shown in Table 7.6. The deterministic ground truths consist of 28 ("Known Answers") out of 23,269 possible answers and the test set resulted in 8 additional "New Answers" (36 answers in total). The results are very similar to query $Q_1(x)$ when comparing the query evaluation with extensional rules only, with the approach that exploits the learned compound relation to partially avoid expensive evaluations of sub-queries with the independent-project rule. Again, the LogLoss score is significantly better, but it is also notable that a really low AUPRC score can be observed for the latter approach (0.0194). From the top 25 ranking of this evaluation method on this query shown in Table 7.7, it can be inferred that the low AUPRC is very likely caused by incompleteness of the corresponding deterministic DBpedia-Music knowledge graph. The answers (rows) that are not highlighted are present in the ground truth generated from the whole data (training set $\cup$ test set). The answers highlighted in green are answers that are true, but are missing in the ground truth. The Hip Hop artists `Xzibit` had a contract with Aftermath/Shady records and was featured on Eminem's Album *The Marshall Mathers LP* among others. For example, `G-Unit` released the EP *G-Unit Radio Vol One* that was produced by Shady

Table 7.6: AUPRC, AUROC and LogLoss scores for evaluating $Q_2(x)$ on DBpedia-Music: *Which musical artists from the Hip Hop music genre involved in a single that was produced by Shady, Aftermath or Death Row records?* Compared are three different evaluation procedures for the query. **Extensional** denotes the evaluation based on pure extensional query evaluation, where RESCAL is used to generate the probabilities. **Learned** additionally approximates sub-queries to avoid evaluations through the independent-project rule. **Random** denotes a ranking of random probabilities. We further compare the answers of these methods against three different set of answers which a described in the column **Ground Truth**.

Evaluating $Q_2(x)$ (RESCAL)

Ground Truth	Evaluated with	AUPRC	AUROC	LogLoss
Known Answers *(Training set)*	**Extensional** *query rules only*	0.4358	0.9512	1.0360
	Learned *compound relation*	**0.6817**	**0.9914**	**0.0745**
	Random *answer*	0.0013	0.5	1.0015
All Answers *(Test set ∪ Training set)*	**Extensional** *query rules only*	0.4258	0.9494	1.0331
	Learned *compound relation*	**0.5999**	**0.9612**	**0.0741**
	Random *answer*	0.0016	0.5	1.0013
New Answers *(All Answers \ Known Answers)*	**Extensional** *query rules only*	**0.3769**	**0.9420**	1.0448
	Learned *compound relation*	0.0194	0.8542	**0.0839**
	Random *answer*	0.0022	0.5	0.9970

Records. `RBX` had contracts with Aftermath Entertainment and Deathrow Records and is featured on the debut album of the rapper Snoop Dogg. The answers highlighted in yellow are answers that are not true, but are also not absurd. `Raekwon` signed a contract with Aftermath Entertainment but the planned album *Only Built For Cuban Linx... Pt. II* was postponed and released later from another record label. `N.W.A` is only partially true since some of its band members, namely `Dr. Dre` and `Ice_Cube` are included in the ground truth answer pool. `Rick_Ross` seems to be the only Hip Hop artist who never had a contract with one these record labels, but he was featured on multiple albums that were produced by Interscope Records; Aftermath Entertainment is part of Interscope Records.

Evaluation of Query $Q_3(x)$

The evaluation results of query $Q_3(x)$, *Which musical artists from the Hip Hop music genre are associated with musical artists that have/had a contract with Interscope Records and are involved in an album whose first letter is a "T"?*, are shown in Table 7.8. The deterministic ground truths consist of 35 ("Known Answers") out of 23,269 possible answers and the test set resulted in 32 additional "New Answers" (67 answers in total).

Table 7.7: Top 25 ranked answers produced by evaluating query $Q_2(x)$ with learned compound relations. The first column is the ranking index, the second the computed probability and the third column holds the answer entities. The rows highlighted in green are correct answers which are not present in the ground truth. Rows marked in yellow denote answers that are fuzzy, but partially true. Red rows indicate wrong answers. Rows that are not highlighted are part of the ground truth.

Index	Probability	Answer Entity
1	1.0	http://dbpedia.org/resource/The_Game_(rapper)
2	1.0	http://dbpedia.org/resource/50_Cent
3	1.0	http://dbpedia.org/resource/Snoop_Dogg
4	1.0	http://dbpedia.org/resource/Eminem
5	1.0	http://dbpedia.org/resource/Dr._Dre
6	1.0	http://dbpedia.org/resource/Nate_Dogg
7	1.0	http://dbpedia.org/resource/Lil_Wayne
8	0.999999999994	http://dbpedia.org/resource/Tha_Dogg_Pound
9	0.999999996251	http://dbpedia.org/resource/Xzibit
10	0.999999991058	http://dbpedia.org/resource/Outlawz
11	0.999999988918	http://dbpedia.org/resource/Kendrick_Lamar
12	0.99999994572	http://dbpedia.org/resource/Akon
13	0.999999884401	http://dbpedia.org/resource/Stat_Quo
14	0.999999795433	http://dbpedia.org/resource/Ice_Cube
15	0.999999742962	http://dbpedia.org/resource/D12
16	0.999999518562	http://dbpedia.org/resource/Lloyd_Banks
17	0.999998715023	http://dbpedia.org/resource/Cashis
18	0.999988920703	http://dbpedia.org/resource/N.W.A
19	0.999986804569	http://dbpedia.org/resource/Mark_Batson
20	0.999983339586	http://dbpedia.org/resource/Kurupt
21	0.999978967051	http://dbpedia.org/resource/Young_Buck
22	0.999973330498	http://dbpedia.org/resource/G-Unit
23	0.999971504099	http://dbpedia.org/resource/Raekwon
24	0.999958233629	http://dbpedia.org/resource/Rick_Ross
25	0.999933133205	http://dbpedia.org/resource/RBX

In difference to query $Q_1(x)$ and $Q_2(x)$, the answers derived through pure extensional query evaluation on the probabilities generated by RESCAL are ranked better against both, "Known Answers" and "New Answers" than the other approach ("Learned"). "Extensional" reaches 0.4811 in AUPRC on the answers derived from the training set and 0.2869 in AUPRC on the new answers that could only be produced by combining all triples from the test and training set. The "Learned" approach that approximates sub-queries

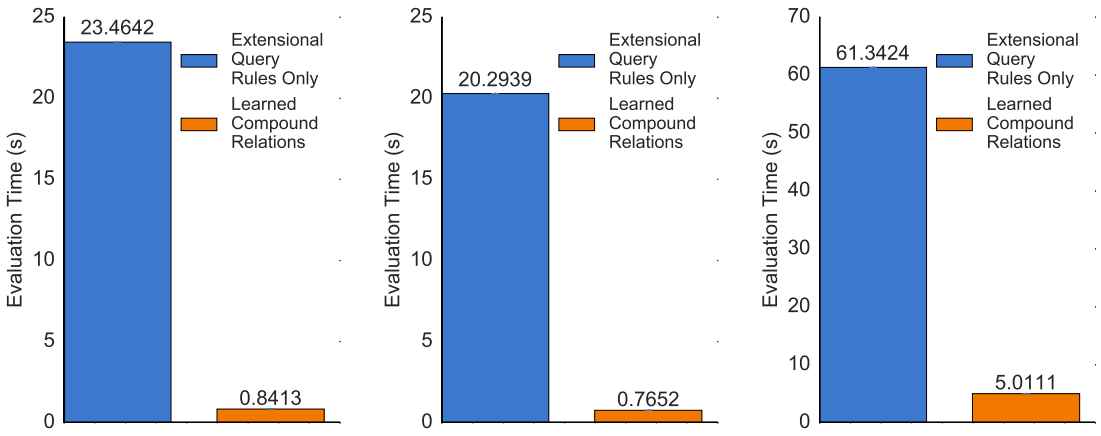
Table 7.8: AUPRC, AUROC and LogLoss scores for evaluating $Q_3(x)$ on DBpedia-Music: *Which musical artists from the Hip Hop music genre are associated with musical artists that have/had a contract with Interscope Records and are involved in an album whose first letter is a "T"?* Compared are three different evaluation procedures for the query. **Extensional** denotes the evaluation based on pure extensional query evaluation, where RESCAL is used to generate the probabilities. **Learned** additionally approximates sub-queries to avoid evaluations through the independent-project rule. **Random** denotes a ranking of random probabilities. We further compare the answers of these methods against three different set of answers which a described in the column **Ground Truth**.

Evaluating $Q_3(x)$ (RESCAL)

Ground Truth	Evaluated with	AUPRC	AUROC	LogLoss
Known Answers *(Training set)*	**Extensional** *query rules only*	**0.4811**	0.9592	1.0314
	Learned *compound relations*	0.4303	**0.9888**	**0.3839**
	Random *answer*	0.0015	0.5	0.9999
All Answers *(Test set ∪ Training set)*	**Extensional** *query rules only*	**0.3957**	0.9076	1.0234
	Learned *compound relations*	0.3320	**0.9632**	**0.3773**
	Random *answer*	0.0029	0.5	1.0007
New Answers *(All Answers \ Known Answers)*	**Extensional** *query rules only*	**0.2869**	0.8499	1.0396
	Learned *compound relations*	0.1589	**0.9338**	**0.3930**
	Random *answer*	0.0014	0.5	0.9965

by learning the compound relation-types reaches only 0.4303 and 0.1589 in these cases. Nevertheless, as in the case of $Q_1(x)$ and $Q_2(x)$, the LogLoss score is significantly better for this approach. By approximating the sub-queries, a LogLoss score of 0.3839 could be achieved when compared against the "Known Answers" and 0.3930 when compared against the "New Answers". Note that the answers generated by the pure extensional query evaluation result in very bad probability values that have a similar LogLoss score as random probabilities (1.0314 for "Known Answers" and 1.0396 for "New Answers"). As in the case of the other queries, we can argue that the answers generated by exploiting learned compound relations in addition to extensional query evaluation are of much higher quality than the answers generated from the pure extensional query evaluation. The ranking (AUPRC) of the former approach is worse than the ranking of the latter, but since it produces much more meaningful probabilities (measured by the LogLoss score), the recognition of uncertain answers is facilitated.

7.4.5 Learned Compound Relations Decrease Query Evaluation Time



(a) Evaluation Time $Q_1(x)$ (b) Evaluation Time $Q_2(x)$ (c) Evaluation Time $Q_3(x)$

Figure 7.4: Query evaluation times in seconds for queries $Q_1(x)$ (a), $Q_2(x)$ (b) and $Q_3(x)$ (c). The blue bars (*Extensional Query Rules Only*) always denote an evaluation of the query using pure extensional query evaluation on the probabilities generated by the latent variable model (RESCAL). The orange bars (*Learned Compound Relations*) also denote an evaluation by extensional query evaluation, but where the application of independent-project rules is partially avoided in sub-queries by approximating these sub-queries through learned compound relations. The evaluation time was measured with an Intel(R) Xeon(R) CPU E7-4850 v2 (OpenBLAS, 24 threads)

In Figure 7.4 the evaluation times in seconds for query $Q_1(x)$ (a), $Q_2(x)$ (b) and $Q_3(x)$ (c) are shown. The blue bars always represent the evaluation of the query on probabilities derived through modeling the knowledge graph with RESCAL with pure extensional query evaluation rules. The orange bars on the other hand represent the second approach that approximates sub-queries by learning compound relations with RESCAL. Thereby the computation of the independent-project is partially avoided. Clearly, the evaluation by the second approach, which exploits these learned compound relations, is 12-27 times faster than the first approach which exploits solely extensional query evaluation rules. For the first two queries, the approximation of sub-queries leads to a decrease in evaluation time from approximately 20 seconds (23.4642 seconds for $Q_1(x)$ and 20.2939 for $Q_2(x)$) to less than one second (0.8413 seconds for $Q_1(x)$ and 0.7652 for $Q_2(x)$). For query $Q_3(x)$ the runtime is decreased from 61 seconds to 5 seconds.

A Comment on the Difference in Evaluation Time of Extensional Query Evaluation in Comparison to the Publication "Querying Factorized Probabilistic Triple Databases"

In [57], we reported much larger evaluation time for query $Q_3(x)$ when evaluating this query solely through extensional query evaluation rules. In fact, we reported that this query remained unanswered after 6 hours. It might be surprising that we reported in the previous section that this query is answered by the same evaluation procedure in 61 seconds.

This large difference in evaluation time is caused by different algorithms that were used to compute the independent-project rule. In [57], we made the restriction that it should be possible to evaluate the query on commodity hardware. For this reason we avoided any materialization of whole relation-types leading to a dense (type-constrained) frontal slice of the tensor. In most of the knowledge graphs there exist relation-types that are unbounded, meaning that domain or range constraints are defined over `owl#Thing`. For large knowledge graphs which contain millions of entities, a materialization of this kind of relation-types from the learned latent variable model becomes quickly intractable due to the huge amount of values (probabilities) that are computed (one for each possible triple). To avoid this explosion in memory we can compute $Q_3(x)$ step by step or block-wise, but this will lead to a significant increase in computation time. In [57], we report the evaluation times based on this memory saving algorithm.

In the previous section, we discarded this restriction and materialized whole relations to compute the queries, i.e. the evaluation through independent-project rule, much more efficiently. It has to be kept in mind that this approach would need a very powerful computer system for larger knowledge graphs and can even then be intractable. Even more impressive, the proposed approach, which partially avoids the evaluation through the independent-project rule by learning compound relations (exploiting intrinsic features of the a priori learned latent variable model), is still magnitudes (12-17 times) faster in evaluating the studied queries than the purely rule based evaluation.

7.5 Related Work

Probabilistic databases (PDB) have gained much interest in recent years and an overview over the state of the art is provided by [100]. Important ongoing research projects include the MayBMS project [47] at Cornell University, the MystiQ project [13] at the University

of Washington, the Orion project [97] at the Purdue University, and the Trio project [75] at the Stanford University. The idea of materialized views on PDBs has been developed in [23], where it was proposed to materialize probabilistic views to be used for query answering at runtime.

Uncertainty in Semantic Web ontologies has been addressed in BayesOWL [24] and OntoBayes [115]. Furthermore, PR-OWL [21] is a Bayesian Ontology Language for the Semantic Web. The link between PDBs, Description Logic and Semantic Web data structures has been explored by [38, 15, 70]. In contrast to these approaches, we start with a deterministic triple store and then derive probabilities via the factorization. Common to all these approaches is the challenge of efficient querying.

In this chapter and in [57] we performed a probabilistic ranking of candidate query answers as done by the top-k querying approaches [27, 84, 95]. However, in difference to these approaches we are pruning low-confidence answers. In these top-k querying approaches, the computation of exact probabilities for the potential top-k answers are avoided by using lower and upper bounds for the corresponding marginal probabilities. Unfortunately, none of these approaches, apart from [27], can avoid extensive materializations in finding answer candidates [103].

As discussed in Chapter 4.4, tensors and other latent variable models have been applied to Web analysis, especially in the context of link-prediction. Link-prediction can be seen as querying a statistically modeled knowledge graph for ground triples. In [83], the YAGO ontology was factorized and meaningful predictions of simple triples in selected subgroups of YAGO were derived through the reconstruction from the low rank representation of the triple store. In this sense, [9, 25, 99] also applied their models for the evaluation of independent triples, but never addressed complex querying on the predictions. In this chapter and [57], we study the significantly more difficult problem of complex querying with predicted triple confidence values (including existentially quantified variables). In this regard, we realize extensional query evaluation on safe queries which can induce complex dependencies between individual predicted triple probabilities throughout the database. In particular, we are concerned with how these queries can be executed efficiently, without the need for extensive materialization of probability tables, by exploiting the factorized representation during querying. In difference to [57], we additionally exploit type-constraints of relation-types when modeling the knowledge graph and during query evaluation. It was shown in the Chapter 5 and [54, 17, 56] that latent variable models generally benefit to a large extent from such prior knowledge on relation-types.

7.6 Conclusion

In this chapter we have demonstrated that knowledge graphs that are statistically modeled with latent variable models can be interpreted as probabilistic databases and can be queried by exploiting the probabilities generated by these models. This approach goes clearly beyond querying for ground triples which is basically performed when applying these models for link-prediction. In this context, we focused on safe queries which can be evaluated in polynomial time by extensional query evaluation rules. We used latent variable models to represent probabilities for a huge amount of triples very efficiently, since it is intractable to explicitly represent the probabilities for every possible triple (considering type-constraints) of the knowledge graph. As a drawback, the probabilities have to be computed "on the fly" when evaluating the queries, which causes additional computational overhead. This computational overhead can be especially severe if sub-queries have to be evaluated using the independent-project rule. We showed that the evaluation of sub-queries through the independent-project rule can be partially avoided by predicting compound relations from the initial deterministic knowledge graph with the pre-trained latent variable model. In our first set of experiments, we gave empirical poof that the evaluation of sub-queries of the form $Q(x, z) : -L_1(x, y), L_2(y, z)$, using the extensional query evaluation rules or using the predicted compound relation $L_3(x, z)$, results in a similar ranking of probabilities. We further applied both approaches for querying DBpedia-Music, a sub-graph of DBpedia which contains entities and relation-types that are related to music. From the experimental result, we can conclude that the approximation of sub-queries through predicted compound relations has many advantages over the evaluation of the queries with pure extensional evaluation rules. First, the query evaluation time is reduced by multiple factors, even when disregarding memory consumption aspects (which lead to faster computations) when evaluating by the independent-project rule. Furthermore, the learned memory efficient representation of the compound relation-types can be stored and used as precomputed views to further decrease query evaluation time in subsequent queries. Second, it results in significantly more meaningful probabilities for the derived answers for the various queries. This observation is particularly interesting, because it allows a more reliable identification of uncertain answers. Third, the approximation of sub-queries through predicted compound relations avoids numerical problems when applying the independent-project rule, where a product of a large number of probabilities has to be computed. In general, the approach is not restricted to the $\exists x.Q$ type queries, but can always be employed when views can be used to simplify the probabilistic query.

Chapter 8

Conclusion

8.1 Summary

In this work, we have studied the application of latent variable models for the statistical modeling of large knowledge graphs. The statistical modeling of these graphs plays an important role in tasks related to completion and cleansing, but also for the automatic construction of knowledge graphs from unstructured textual data. Due to their size, large knowledge graphs are especially challenging to model because they introduce additional constraints on the statistical model, i.e. limiting the complexity of the embedding space of the latent representations for relation-types and entities. Enforcing large embeddings to increase the expressiveness of latent variable models will inevitably lead to very long to intractable training times and high memory consumption when exploiting them for these graphs. For this reason, it has to be considered that the latent variable models have to be parsimonious in their number of parameters to be tractable. Examples include Google's Knowledge Vault system, where the used neural network exploits latent embedding vectors of length no more than 60 to model the entities and relation-types of Freebase, which has millions of entities and thousands of relation-types. Throughout this work, we have considered three different latent variable models that cover the current state of the art in scalable latent variable models for the statistical modeling of large knowledge graphs. The first, RESCAL, is a very efficient third order tensor factorization method which exploits the natural representation of triples in a third-order tensor. The second, Translational Embeddings (TransE) model interprets triples as translations in the latent embedding space, and the third, mwNN is the earlier mentioned multiway neural network approach used in the Google Knowledge Vault system.

In our initial experiments presented in Chapter 4, we compared these models under the constraints imposed by large knowledge graphs. From these experiments, we observed that the prediction quality of all three models on selected data sets from Freebase, DBpedia and YAGO was often of moderate quality when these models are limited in their complexity. TransE clearly achieved the highest prediction quality in the link-prediction tasks when compared with the other two models, but RESCAL is clearly superior in terms of training times and it has a low number of hyper-parameters, decreasing model tuning effort to a minimum. The multiway neural network model (mwNN) resulted in a similar link-prediction quality than RESCAL, but with significantly longer training times. This model is also the most complex one in terms of hyper-parameters, resulting in a high effort for hyper-parameter tuning.

It is intractable to generally increase the dimensionality of the latent embeddings for entities and relation-types to improve the expressiveness of latent variable models when modeling large knowledge graphs. For this reason we require a different approach to reduce the complexity of the modeling tasks that will empower the latent variable models to focus on the important aspects of the data. We showed in Chapter 5 that prior knowledge on relation-types in form of type-constraints, as provided by the schema of knowledge graphs, is one effective way to reduce this complexity with great impact on the modeling quality. For all three latent variable models and a diverse set of triple data extracted from Freebase, DBpedia and YAGO, we were able to observe improvements up to 77% in link-prediction quality in terms of Area Under Precision Recall Curve. Due to the many aspects in which these models differ and the fact that they have been the major targets for extensions from multiple research groups around the globe, we further argue that the observed improvements are not limited to the studied three models (RESCAL, TransE and mwNN), but that the integration of prior knowledge on relation-types is of general value to latent variable models when modeling knowledge graphs. In addition, we could observe similar large improvements when exploiting a local closed-world assumption on relation-types instead of type-constraints. The great advantage of this local closed-world assumption lies in the fact that it is independent from any prior knowledge about the knowledge graph's schema, but is solely based on observed triples in the graph. We could not observe from our experiments that the integration of the local closed-world assumption leads to generally better results than the integration of curated type-constraints into the latent variable models. For this reason, the local closed-world assumption should be applied on those relation-types where type-constraints are missing or fuzzy. In difference to type-

constraints, the local closed-world assumption can also be applied to schema-less knowledge graphs.

Besides improving models individually, a different way to improve link-prediction is to combine diverse predictors in ensemble methods. We have provided and discussed empirical proof in Chapter 6 that due to their large amount of differences, RESCAL, TransE and mwNN are well suited for combination in an ensemble solution for link-prediction in large knowledge graphs. In the conducted experiments the ensemble always resulted in superior prediction quality with improvements of up to 15% on top of the improvements achieved through the integration of type-constraints in the individual models. Especially TransE was observed to learn different aspects of the data than RESCAL or mwNN and the combination of the TransE with the other two models resulted in the largest improvements over the best single predictor incorporated in the ensemble. These improvements were observed to be especially large when the models exploited very low dimensional embedding for entities and relation-types, where the ensemble method achieved a similar performance as the best single predictor that was allowed to exploit 10 times higher dimensional embeddings.

When applying latent variable models to knowledge graphs for link-prediction, this is basically a singular event. We model the given deterministic knowledge graph once and extract the triple confidences which are exploited for complementing or cleaning the triples in the graphs in a follow up step, and discard the model afterwards. In Chapter 7, we described a new interpretation of the trained statistical model as probabilistic database which extends its application beyond predicting confidences for ground triples. This new interpretation allows us to exploit the theory of probabilistic databases for complex probabilistic querying of these graphs. Since it is intractable to pursue the naive approach, where we materialize all possible triple probabilities and simply apply probabilistic rules for query evaluation, we showed that an alternative approach, which recycles the learned latent representations of entities and relation-types, makes probabilistic safe querying tractable on statistically modeled large knowledge graphs. As a drawback, this alternative approach introduces additional computational load which can lead to significantly increased query evaluation times, even though the queries are safe and especially if the independent-project-rule on a large amount of entities is applied. We proposed to learn compound relations by exploiting intrinsic features of the latent variable model and showed that the learned compound relations lead to very good approximations of an instead applied independent-project-rule decreasing the total query evaluation time dramatically (12-27 times faster). Furthermore, these learned compound relations avoid numerical issues that can arise when

the independent project rule is applied on a large set of probabilities. In our experiments, where we queried the music domain of DBpedia, the evaluation approach which combines extensional query evaluation rules with learned compound relations resulted in clearly more meaningful probabilities for the produced answers.

8.2 Future Directions and Applications

Knowledge graphs are of great value for a wide set of applications today, but they also suffer from many deficiencies. Especially incompleteness is one of the major problems in these graphs that can only be tackled with the support of reliable automated approaches. For this reason, there is a high demand for statistical models which support in applications such as knowledge graph construction, completion and cleaning, but also for dealing with uncertainties. Latent variable models have proven to be well suited for the modeling of knowledge graphs, but due to the limitations imposed by the size of large knowledge graphs, we belief that these models have to be combined with prior knowledge on the graph or its structure to unfold their full potential. The integration of prior knowledge about relation-types lead to improved low dimensional embeddings of entities and relation-types that are of interest for tasks related to disambiguation and link-based clustering in large scale applications.

Furthermore, there are many aspects in which RESCAL, TransE and KVNN differ (see discussion in Chapter 3.3) and which have to be analyzed more deeply. Identifying these models' key aspects that have the most beneficial impact on link-prediction quality can give rise to a new generation of latent variable approaches that could further drive knowledge-graph modeling. Nevertheless, we expect that it will be very difficult for the current state of the art latent variable models to capture the complete underlying structure and dependencies of the whole knowledge graph under the complexity limits imposed by large knowledge graphs on the embedding space. The combination of latent variable models with graph-feature models as proposed by [25, 80] or the combination of diverse models of low complexity as proposed in this work offer an efficient way to increase link-prediction quality. Unfortunately, these ensemble methods will not result in better embeddings for entities or relation-types which are of major interest for various applications that rely on embeddings reflecting the semantics of entities and relation-types. A possible solution to this problem is offered by Deep Learning approaches where the complexity of the learning task can be covered by a hierarchy of neural network layers that result in latent features

that reflect more complex dependencies observed in the graph. In contrast to the other latent variable approaches, the deeper layers in the neural network hierarchy are not directly dependent on the size of the knowledge graph as the first embedding layer and will therefore not necessarily explode in the amount of parameters. A potential successful application of Deep Learning for link-prediction in knowledge graphs is currently an open research question, but very promising.

Additionally, in some cases the truthfulness of a triple might not only be dependent on single ground triples, as considered by the latent variable models discussed in this work, but on complex associations of facts that actually represent whole paths in the knowledge graphs (e.g. nested facts). It might be beneficial to consider these paths in a whole and not as a composition of independent atomic triples when modeling the knowledge graphs [77, 40]. Models that are able to additionally consider these paths are of special interest for querying knowledge graphs and could further complement the probabilistic querying of knowledge graphs proposed in Chapter 7.

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