Bachelor’s Thesis

Feature Learning for Meta-Paths in Knowledge Graphs

Feature Learning für Meta-Pfade in Wissensgraphen

Sebastian Bischoff
sebastian@salzreute.de

Submitted on July 30, 2018

Knowledge Discovery and Data Mining Group
Hasso Plattner Institute, Germany

Supervisors
Dr. Davide Mottin
Prof. Dr. Emmanuel Müller
Abstract

In this thesis, we study the problem of feature learning on heterogeneous knowledge graphs. These features can be used to perform tasks such as link prediction, classification and clustering on graphs. Knowledge graphs provide rich semantics encoded in the edge and node types. Meta-paths consist of these types and abstract paths in the graph.

Until now, meta-paths can only be used as categorical features with high redundancy and are therefore unsuitable for machine learning models. We propose meta-path embeddings to solve this problem by learning semantical and compact vector representations of them. Current graph embedding methods only embed nodes and edge types and therefore miss semantics encoded in the combination of them. Our method embeds meta-paths using the skipgram model with an extension to deal with the redundancy and high amount of meta-paths in big knowledge graphs.

We critically evaluate our embedding approach by predicting links on Wikidata. The experiments indicate that we learn a sensible embedding of the meta-paths but can improve it further.
## Contents

1 Introduction 1

2 Related Work 5

3 Meta-path Embedding 9
   3.1 Background ........................................ 10
   3.2 Embedding Model .................................... 11
      3.2.1 Meta-path-based Edge Embedding ............. 12
      3.2.2 Meta-path-based Node Embedding ............. 12
      3.2.3 Node type-based Node Embedding ............. 12
   3.3 Meta-path Mining ................................... 13

4 Evaluation 18
   4.1 Link Prediction in Knowledge Graphs .............. 19
      4.1.1 Node type-based Node Embedding ............. 20
      4.1.2 Meta-path-based Node Embedding ............. 21
      4.1.3 Meta-path-based Edge Embedding ............. 22
      4.1.4 Comparison with Node Embedding Methods .... 23
   4.2 Future Experiments .................................. 24
      4.2.1 Does the Embedding Capture the Concepts Which
           the Meta-paths Represent? ..................... 24
      4.2.2 Link Type Prediction in Knowledge Graphs ... 25
      4.2.3 Knowledge Graph Completion ................. 26

5 Implementation Details 27

6 Conclusion 28

7 Acknowledgements 29

References 31
1 Introduction

The research community showed an increased interest in knowledge graphs over the last years. They are able to structure large amounts of information and can therefore be used in various domains and use cases. One well-known and daily used application is in Google’s search for entity disambiguation, enrichment of search results and exploratory search [60]. A knowledge graph could also be used as a source of knowledge for a future AI system. How to provide general knowledge to such a system is one of the problems of AI [41].

Firstly, knowledge graphs or information networks are a very general way of storing information. Therefore, methods that are based on them are generally applicable independent of the data or the domain. Secondly, different fields use them for collecting information. Biologists for example are building protein-protein interaction networks or gene regulatory networks to investigate the workings of proteins and genes. Most of the data on the web is unstructured [11]. To make these resources usable, different approaches were proposed to extract knowledge graphs from unstructured data sources such as Wikipedia [73] or the web. Lastly, they can be used to combine information from multiple sources in the process of information fusion [70].

Such knowledge graphs can be used to perform tasks such as classification, prediction, clustering or anomaly detection. The usefulness of these tasks depends on the data and the meaning in the domain. The prediction of missing links, also called knowledge base completion, can help to suggest friends in a social network or to reduce the experimentation costs in biology. Molecular interactions can be modeled as a link prediction problem on a corresponding graph. Because 99.7% of these interactions in human cells [72, 4] are still unknown [48], it would be helpful to focus the experiments on interactions with a high probability. Another type of link prediction is the one where we want to predict future links in an evolving graph. Concerning nodes, we can classify them in predefined classes, cluster them in groups with similar characteristics, detect anomalies [3], rank them for information retrieval [70], and recommend them to a user.

All current methods focus on embedding only nodes or nodes and edge types simultaneously. To the best of our knowledge no other work proposes node type embeddings except Xie et al. [91] who learn multiple embeddings per type. All the other publications work with triplets (head entity, relation, tail entity), not including node types. Furthermore, there is no method for embedding meta-paths. Meta-paths are sequences alternating node and edge types. They are an abstraction of paths in the underlying graph and therefore summarize many paths.
Methods for future link prediction based on meta-paths [77, 92] only use structural features and no semantic features.

However, knowledge graphs contain much richer information that is not used by the previously mentioned methods. By representing specific concepts in the domain, meta-paths are capturing semantics which can not be represented when considering nodes and edges alone. The correlation of meta-paths is more meaningful than the correlation of edges and nodes. So one would expect a higher predictive power with meta-paths as features. Furthermore, meta-paths span more than only the direct neighborhood and hence yield features with more information. They extend over the direct neighborhood with the cost of a high time complexity when computing them.

The main problem is that meta-paths consist of categorical entities, namely node and edge types. Almost all machine learning algorithms need vector representation of the input data. The simplest way to transform meta-paths into vectors would be to encode them with an ID in the form of a one-hot representation. The problem with this representation is that the number of meta-paths is exponential in the length of the meta-paths and the dimensionality grows linearly with the number of meta-paths. Therefore, all machine learning algorithms will suffer from the curse of dimensionality. Additionally, meta-paths are highly redundant because of the shared subparts and therefore this representation contains a lot of redundancy.

The need for vector representations of texts arose early in the data mining and information retrieval community. They are needed for document classification, document retrieval, and document ranking. The first approaches represented words by a combination of latent classes learned from an underlying text corpus [20, 33, 10]. Afterwards, the focus shifted to learning vector representations by optimizing a prediction based loss [52, 53]. The assumption in these embeddings is that words occurring together in a context share some form of meaning [31].

We have to make some assumptions to use the methods developed in the text embedding community for meta-path embeddings. We assume that meta-paths which occur in the same context also share some form of meaning. The context is defined by all the meta-paths between two nodes. If we take two actors that played together in a movie, played in different episodes of one TV series and went to the same (acting) school, then their nodes are connected by meta-paths representing these concepts. All these concepts share at least the "dimension" acting but maybe there are also other ones present such as occupation and education.
Scope and limitations  Prerequisite for our method is that edge and node types are defined on the knowledge graph. There are knowledge graphs that do not satisfy this requirement but there are also many schema-based knowledge graphs such as Freebase, Wikidata, DBpedia, YAGO and Google Knowledge Graph that can be used. They do not necessarily have to provide a node type directly. It is sufficient that a class hierarchy is defined in the knowledge graph and that each node has an instance of-relation with a class. If meta-paths are given on a graph, we can compute embeddings for them in a reasonable time. If meta-paths and their embeddings are only an intermediate step, one major drawback of our approach is that meta-paths are expensive to compute. However, we do not need all meta-paths on the graph and we therefore propose a probabilistic mining algorithm with a reduced runtime.

Outcomes  Our experiments show that the approach learns a sensible representation of meta-paths and especially their components, node and edge types. However, we have to refine the meta-path-based features for link prediction and perform additional experiments to evaluate our approach more thoroughly.

Contribution  In this work, we propose meta-path embeddings targeting real-world knowledge graphs, node and edge type embeddings, an enhanced version of link prediction based on meta-paths and new vector representations for edges and nodes based on meta-paths. Furthermore, we introduce an experiment stack to mine meta-paths, to transform them for the usage with text embedding implementations and to perform link prediction.

Bachelor Project  In our bachelor project, we built an interactive exploration tool for knowledge graphs motivated by a biological use case of our project partner. The exploration tool incorporates the domain knowledge of a user into the exploration process by querying ratings of meta-paths from the user. As mentioned earlier, the number of meta-paths is very high and exceeds the number of ratings a user wants to provide to the system. To overcome this problem, the system uses active learning to only query ratings for a selection of meta-paths. This selection is based on how much new information the meta-paths provide. Simultaneously, it learns a predictor for the user rating and uses it for all meta-paths the user did not rate. This part requires manual feature engineering or an embedding of the meta-paths. Lastly, the naive computation of meta-paths turned out to be infeasible.
1 Introduction

Structure of the Thesis  In Section 2 we discuss the current body of work related to our approach, in Section 3 we introduce our meta-path embedding model, node and edge embeddings based on the model and a meta-path mining algorithm, in Section 4 we present different experiments to evaluate our approach and compare it with other approaches, in Section 5 we discuss some implementation details, and conclude our work in Section 6.
2 Related Work

The body of work related to our method can be divided in the group of graph embedding on classical graphs and knowledge graphs, text embedding, meta-paths-based works and link prediction. In the following, we briefly summarize the different fields and compare the approaches.

**Meta-paths** Meta-paths [78, 50] were first introduced for the definition of Pathsim [78], a similarity measure on heterogeneous graphs. Later, HeteSim [68, 69] extended Pathsim by allowing to measure the similarity of objects with different types and removing the restriction on symmetric paths. Meta-paths are further used in tasks like user-guided entity clustering [80], link prediction [92, 79, 77], multi-network collective link prediction [94], collective classification [37], entity similarity search [93], and entity ranking [47].

**Node embedding** Methods for node embedding like node2vec [27], DeepWalk [64], LINE [82], VERSE [85], HOPE [62] and GraRep [18] embed the structure of a graph without edge and node types. Graph factorization models [2] use matrix factorization for node embedding.

DeepWalk [64] performs random walks on the graph, it treats walks as sentences and embeds them using the word2vec skipgram model [52, 53]. Similarly, we mine the meta-paths in a random walk fashion and treat meta-paths as words because we embed using the principle that meta-paths in the same context have a similar meaning. Whereas, DeepWalk uses the principle that nodes in the same context have a similar meaning.

**Knowledge graph embedding** When we work with knowledge graphs, we have more information available to embed nodes, edge types and node types. The first group of methods performs node embedding by incorporating the extra information from knowledge graphs. The neighborhood mixture model [58] uses the embedding of neighboring nodes and the connecting edges to calculate a node embedding. It is based on methods which produce node and edge embeddings like TransE [16] and TransH [90]. Metapath2vec [22] embeds after the same principle as node2vec [27]. DeepWalk [64] and LINE [82] does, using the skipgram model. They extend the node embedding methods on simple graphs by proposing a way to incorporate the information in heterogeneous graphs. To achieve this, they condition random walks, producing "sentences", on user-specified meta-paths. One problem with this approach is that the results strongly depend on
the selected meta-path(s) and that the user needs a deeper understanding of the
graph to choose them correctly. They referred in their experiments to other publi-
cations [34, 74, 78, 80] to find the best working meta-paths for tasks on academic
networks. This shows how their experiments specifically target the data sets and
that a more general meta-path-based approach would be favorable. Luo et al. [49]
treat meta-path instances which they call knowledge paths as words and embed
them with the skip-gram model. In a second step, they refine the embedding with
SME [17], TransE [16] or SE [14].

Another body of work learns node and edge embeddings jointly. Garcia-Duran
et al. [24] groups them in two-way approaches and three-way approaches. Two-
way approaches such as SME [17], TransE [16], TransH [90] and TransR [45] model
the interactions between the head and the tail, the head and the label, and the
label and the tail of knowledge graph triplets. Three-way [24] approaches such as
TATEC [24] jointly model the interaction of head, label and tail. Two-way ap-
proaches use vectors and three-way approaches use matrices to model the relation.
All these approaches mainly differ in the parameterization of nodes and edges as
vectors or matrices and their cost function [89]. These works learn only from the
knowledge triplets and therefore do not capture the structure of the graph. Fur-
thermore, they do not explicitly model the node types and can only learn from
them implicitly, if a taxonomy is defined in the triplets they use to learn their
embeddings. It remains an open question how well the node types are captured.
Another line of work uses multi-layer fully connected neural networks [61] and con-
volutional neural networks such as ConvE [21] and ConvKB [59] to map triplets
to an embedding.

Only Xie et al. [91] and Guo et al. [28] use node types in their graph embedding.
Xie et al. [91] learns a projection matrix for each node type, where a node type
has a specific embedding dependent on the relation it occurs in. Guo et al. [28]
proposes a semantically smooth embedding where nodes with the same node types
should be closely located to each other in the embedding space [89].

Another line of work uses relation paths which are like meta-paths but without
node types. They only include edge types. Relation path embedding such as
PTransE [46] tries to embed nodes and relationships in a knowledge graph so that
the combination of relationships is a sensible embedding for the path composed of
this relationships. Toutanova et al. [84] include nodes into the relation paths. In
comparison, node types in the relation path (= meta-path) help us to generalize
because two paths with different nodes but the same node types are learned inde-
dependently by Toutanova et al. [84] and jointly in our method. Path queries [30]
such as What parts of an Airbus A380 are made out of steel? that would translate
to A380 - has_part - part - material_used - steel can be interpreted as relation
paths [57] and if the user would specify node types in their query such as part also
as meta-paths. Consequently, we can use meta-paths to enhance the answering of
path queries.
Table 1: Comparison of different graph embedding methods regarding the objects they embed.

| subset               | Nodes | Node types | Edge types | Meta-paths |
|----------------------|-------|------------|------------|------------|
| Node embedding techniques | [27, 64, 85, 82, 62, 18] | x          |            |            |
| Translational approaches | [16, 90, 17, 14, 45, 46] | x          | x          |            |
| TKRL                  | [91]  | x          | (x)        | x          |
| Neighborhood mixture model | [58]  | x          |            |            |
| metapath2vec          | [22]  | x          |            |            |
| Our method            |       | x          | x          | x          |

Lastly, there are many other works using additional data such as text with mentions of knowledge graph entities [83] for the embedding which improves the performance [81] or using other features from the graph such as subgraphs generated with random walks for knowledge base completion [88]. All these approaches are compared in Table 1.

**Text embedding**  The first text embedding approaches based on latent class models were methods such as latent semantic analysis [20], probabilistic latent semantic indexing [33] and latent dirichlet allocation [10] in the field of distributional semantics [86, 7]. The distributional hypothesis [31] suggests that words in the same context often have a similar meaning. Based on this hypothesis, predictive models were first proposed for embedding words [52, 53] and later also for sentences [39, 29], paragraphs [39], and documents [29]. Another group of approaches uses the matrix factorization of the word co-occurrence matrix [63, 54, 42, 66].

The embedding of sentences and paragraphs with paragraph vectors [39] could be transferred to meta-paths by treating one meta-path as a sentence. This would result in a model which does not take the high redundancy of meta-paths into account and would learn inefficiently.

An addition to the skipgram model [12] uses character n-grams for each word to capture subword information. A word is represented as the sum of the embeddings of n-grams contained in the word.

Even smaller entities are considered in character level language models trained with recurrent neural networks [51, 81, 26] or convolutional neural networks [36]. Other ways to calculate features for texts are based on n-grams or are built by hand with features which are believed to perform well on the specific task.
Link prediction Different tasks using these embeddings were proposed. The task of predicting missing links, named knowledge base completion, got the most attention. All models producing embeddings for nodes such as Unstructured [17] or nodes and edges such as TransE [16] can be used for a scoring function $f(h, t)$ or $f(h, r, t)$ of the plausibility of a knowledge base triplet $(h, r, t)$ [57]. Another task defined on these triplets is triplet classification [71] where a classifier predicts if a given triplet exists in the knowledge graph. The link prediction over evolving graphs was first introduced in the social sciences [43]. It is a harder link prediction problem than in knowledge graph completion because a classifier has to learn the formation mechanisms of links [19] instead of modeling the likelihood of links in a given graph.

Special tasks on academic networks such as DBLP$^1$ are citation and co-authorship prediction. Sun et al. [77] approach co-authorship prediction by searching all meta-paths between authors, calculate structural values for all these meta-paths and then learn a classifier to predict, if two authors will write a paper together in the future. This approach only works for graphs with a small number of node and edge types because otherwise the number of dimensions of the feature space spanned by the meta-paths is very high. Our method does not suffer from this problem because it reduces the number of dimensions. Furthermore, we are not only considering the topology of the graph but also the semantics of the meta-paths. Yu et al. [92] propose a method for citation prediction also based on structural features of meta-paths such as the number of instances. They do not use any semantic features of meta-paths.

An extended version of this problem is the estimation of the point in time a link will occur. Sun et al. [79] mine meta-paths between the two nodes of an edge and calculate different measures based on them as features for a classifier. We also use the meta-paths between two nodes in our meta-path-based edge embedding in Section 3.2.1 but we are using the combined embeddings of the meta-paths, instead of the measures of a meta-path, as features for a relationship building time predictor. We could incorporate the topological features of Sun et al. [79, 77] and Yu et al. [92] as a weighting of the embeddings of the single meta-paths.

The path ranking algorithm [38, 25, 88] uses relation paths as features for tasks like entity ranking. This could be extended by using meta-paths instead of relation paths.

$^1$https://dblp.uni-trier.de
3 Meta-path Embedding

Many different topological features such as common neighbors, preferential attachment [56], *Katz* [35], *Adamic/Adar* [1], and *PropFlow* [44] were proposed for homogeneous networks. Most of them are not usable for heterogeneous networks [79]. Instead, we can use meta-paths as topological features in heterogeneous networks [77] because meta-paths encode topological features [79]. Meta-paths are a very general representation which can even be transferred between graphs, if a mapping of the node and edge types is defined. Meta-paths alone are not sufficient for the definition of these features. We have to use measures such as instance counts and random walks [77] to quantify a meta-path.

A predictor trained with these features lacks any information about the "meaning" of a meta-path because the previous features only concern the structure of a graph. If we would have features describing the semantics of a meta-path, we could combine them with the structural features to get a holistic feature set.

To get these semantical features and overcome the representation of meta-paths as categorical features, we propose meta-path embeddings. By embedding meta-paths, we get a compact representation of the enormous amount of (meta-)paths in real world knowledge graphs. Additionally, we reduce the redundancy in the meta-paths and transform them to a representation machine learning algorithms can easily use.

To derive a meta-path embedding from text embedding approaches, we map the different parts of a word embedding to a graph as follows

- The text corpus equals the whole graph.
- One sentence equals all meta-paths between two nodes. Thereby, defining the context of one meta-path. This definition comes from the assumption that meta-paths which occur in the same context also share some form of meaning. The underlying intuition is that meta-paths which connect the same nodes in a graph are similar.
- One word equals one meta-path.

We deal with the redundancy of meta-paths by using ideas for capturing sub-word information. Bojanowski et al. [12] propose an extension of the skip-gram model [53, 52] by including character-level n-grams into the embedding. This results in an embedding which takes advantage of shared parts in word families. In our case, the parts of a word equal parts of a meta-paths. These parts are combinations of node and edge types which also occur in different meta-paths.
The redundancy of meta-paths is an observed problem which is addressed by Kong et al. [37] with the decomposition of meta-paths in smallest, non-trivial meta-paths. They argue that many, and in part redundant, meta-paths are noise for a classifier. We deal with the redundancy by capturing the subword information and projecting to the embedding space.

In the following parts, we first introduce the necessary definitions for this work, our embedding model, different features for nodes and edges and describe the mining of meta-paths for the embedding.

3.1 Background

In this chapter, we introduce the definition of knowledge graphs, their homogeneity and heterogeneity, meta-paths on the network schema and embeddings.

Definition 3.1 (Knowledge graph [75 76]). A knowledge graph, also named information network, is a directed graph $G = (V, E, \varphi, \psi)$ with a set of node types $\mathcal{A}$ and edge types $\mathcal{R}$. A node type mapping function $\varphi : V \mapsto \mathcal{A}$ maps nodes to their node types and an edge type mapping function $\psi : E \mapsto \mathcal{R}$ maps edges to their edge types. Furthermore, the edge types imply the node types as follows $\psi(e_1 = (v_1, u_1)) = \psi(e_2 = (v_2, u_2)) \implies \varphi(v_1) = \varphi(v_2) \wedge \varphi(u_1) = \varphi(u_2)$ [70].

Definition 3.2 (Homogeneous/heterogeneous knowledge graph). If a knowledge graph has multiple node types $|\mathcal{A}| > 1$ or edge types $|\mathcal{R}| > 1$, we call it a heterogeneous knowledge graph or heterogeneous information network (HIN). We call a knowledge graph a homogeneous knowledge graph, if it has only one node type $|\mathcal{A}| = 1$ and edge type $|\mathcal{R}| = 1$.

Definition 3.3 (Network schema [75 76]). $S_G = (\mathcal{A}, \mathcal{R})$ is a network schema of a knowledge graph $G = (V, E, \varphi, \psi)$.

Definition 3.4 (Meta-path [77 78]). The meta-path associated with the path $\langle n_1, ..., n_t \rangle, n_i \in V, 1 \leq i \leq t$ is a path on the network schema $S_G = (\mathcal{A}, \mathcal{R})$ with length $t$. It is a sequence $\mathcal{P} : (\varphi(n_1), \psi((n_1, n_2)), ..., \psi((n_{t-1}, n_t)), \varphi(n_t))$ that alternates node and edge types along the path [9].

A meta-path instance is a path in the knowledge graph where the nodes and edges have the types specified in the meta-path.

Definition 3.5 (Embedding). An embedding $f : k \rightarrow r$ with embedding size $n$ maps $f : K \mapsto \mathbb{R}^n$. A meta-path embedding $\text{emb} : mp \rightarrow r$ therefore maps $\text{emb} : \mathcal{MP} \mapsto \mathbb{R}^n$. 
3.2 Embedding Model

Our model and formalization follows Bojanowski et al. [12] but is adapted to meta-paths. We have a meta-path vocabulary $MP$ of size $|MP|$ and denote each meta-path by its index $mp \in 1, ..., |MP|$. Our goal is to learn a vector representation for each $mp$. The skipgram model needs a training corpus of size $T$ denoted as $mp_1, ..., mp_T$. The training objective of the skipgram model is to maximize the probability of the meta-paths in the context given the meta-path given by

$$
\sum_{t=1}^{T} \sum_{c \in C_t} \log p(mp_c|mp_t)
$$

$C_t$ being the context of the meta-path with index $t$ and $c$ is one meta-path in the context. The context is defined as a subset of all meta-paths between two nodes. With $m$ meta-paths between two nodes and the equivalent of a sentence being $n$ meta-paths long, we have $\binom{m}{n}$ possible sentences because the graph does not define a order of the meta-paths. In real world knowledge graphs, $m$ is rather high and the therefore resulting high number of sentences causes a need to sample from them.

We then express the prediction of the meta-paths in the context $C$ as binary classification tasks with the logistic loss function $l : x \mapsto \log(1 + e^{-x})$ and a set $n \in \mathcal{N}_{t,c}$ of negative examples drawn randomly from the the vocabulary $MP$ which results in the objective

$$
\sum_{t=1}^{T} \left[ \sum_{c \in C_t} l(s(mp_t, mp_c)) + \sum_{n \in \mathcal{N}_{t,c}} l(-s(mp_t, n)) \right]
$$

Now, it only remains to define the scoring function $s$. We use the embedding vectors $v_{mp_t}$ of the currently selected meta-path and the one of the meta-path in the context $v_{mp_c}$ and define $s(mp_t, mp_c) = v_{mp_t}^\top v_{mp_c}$.

We could embed meta-paths only with the skipgram model but this would not address the redundancy of them. For this reason, subword information is added to the skipgram model. The subword information is captured by an embedding of n-grams. In the extended model, we additionally have a dictionary of n-grams $G$ with $min \leq n \leq max$ where $min$ is the minimal length and $max$ the maximal length of n-grams in $G$. The n-grams in meta-path $mp$ are denoted as $G_{mp}$. We define the scoring function $s(mp, c)$ in the subword model as

$$
s(mp, c) = \text{emb}(mp)^\top \text{emb}(c)
$$
Furthermore, the embedding of one meta-path is defined as
\[
\text{emb}(mp) = \sum_{g \in \text{G}_{mp}} \text{emb}(g)
\]
This also produces node type \( \text{emb}_{\text{nodetype}}(i) \) and edge type \( \text{emb}_{\text{edgetype}}((i,j)) \) embeddings, if we choose \( \text{min} = 1 \). We would not expect a very good performance in comparison with future methods specifically designed for node type embeddings. These embeddings are the baseline version of our method. Based on this model, a definition of different node and edge representations is possible.

### 3.2.1 Meta-path-based Edge Embedding

An edge \( u = (i,j) \) can be represented by all the meta-paths connecting nodes \( i \) and \( j \). Given \( i, j \in V \), \( \mathcal{MP}(i,j) \) is defined as all meta-paths between nodes \( i \) and \( j \) and \( \text{emb}_{\text{edge}} : E \mapsto \mathbb{R}^n \) as edge embedding function. The representation of the edge \( (i,j) \) is defined as
\[
\text{emb}_{\text{edge}}((i,j)) = \frac{1}{|\mathcal{MP}(i,j)|} \sum_{mp \in \mathcal{MP}(i,j)} \text{emb}(mp)
\]

### 3.2.2 Meta-path-based Node Embedding

Given \( i \in V \), \( \mathcal{MP}(i) \) is defined as all meta-paths starting or ending in node \( i \) and \( \text{emb}_{\text{node:mps}} : V \mapsto \mathbb{R}^n \) as node embedding function. The representation of node \( i \) is defined as
\[
\text{emb}_{\text{node:mps}}(i) = \frac{1}{|\mathcal{MP}(i)|} \sum_{mp \in \mathcal{MP}(i)} \text{emb}(mp)
\]

### 3.2.3 Node type-based Node Embedding

We extend \( \varphi \) to \( \varphi'(i) \), \( \varphi' \) returns the set of node types of node \( i \). Given \( i \in V \) and \( j \in \varphi'(i) \), \( \text{emb}_{\text{nodetype}}(j) \) is defined as embedding of node type \( j \). The embedding of the node types is defined as \( \text{emb}_{\text{nodetype}} : \mathcal{A} \mapsto \mathbb{R}^n \) and the embedding of one node based on its node types is defined as \( \text{emb}_{\text{node:nodetypes}} : V \mapsto \mathbb{R}^n \). The representation of node \( i \) is defined as
\[
\text{emb}_{\text{node:nodetypes}}(i) = \frac{1}{|\varphi(i)|} \sum_{u \in \varphi(i)} \text{emb}_{\text{nodetype}}(u)
\]
One could further add a parameter to this definition weighting the depth of the node type in the class hierarchy. With this parameter, one could give more weight to fine-grained classes because they cover the details of a node.

Liben-Nowell and Kleinberg \[43\] state that it is not sensible to predict edges where one of the nodes is not present in the training data. In principle, we can produce embeddings for any nodes, if the node types of the new nodes are provided and present when training the embedding.

We could further define an individual node embedding by first embedding all nodes with their node types and then learning a delta to represent the specific characteristics of each node. Given \( u \in V \), \( \sum_{w \in \varphi'(u)} \text{emb}_{\text{nodetype}}(w) \) is defined as the embedding of the node types \( \varphi'(u) \) of \( u \) and \( \text{emb}_\Delta(u) \) as the embedding of only node \( u \). \( \text{emb}_{\text{node}:\text{delta}}(u) \) as the embedding of \( u \) is defined as

\[
\text{emb}_{\text{node}:\text{delta}}(u) = \sum_{w \in \varphi'(u)} \text{emb}_{\text{nodetype}}(w) + \text{emb}_\Delta(u)
\]

### 3.3 Meta-path Mining

If no meta-paths are given, we have to calculate them. In the following, we introduce our algorithm, demonstrate its problems and propose an improved version.

Generally, the graph is treated as undirected and the following algorithms assume that each node has only one node label. The algorithm can easily be extended to multiple types per node by collecting the types along the meta-path and forming the cartesian product in the end.

The parameters for Algorithm 1 are a knowledge graph \( KG = (V,E,\varphi,\psi) \) consisting of a graph \( G = (V,E) \) with node labeling function \( \varphi \) and edge labeling function \( \psi \) and \( \text{metaPathLength} \) specifying the maximum meta-path length. The algorithm works in a breadth-first manner and calls the function \( \text{computeMetaPaths} \) for each node in the graph.

Function \( \text{computeMetaPaths} \) additionally gets the \text{metapath} up to this point, start node \( u \) and current node \( v \) as input. It saves the meta-path which is extended by the label of the current node as a meta-path between the start node and the current node. Afterwards, it recursively calls itself for each edge of the current node after adding the edge label to the meta-path.
Algorithm 1: Meta-Path Mining

**input:** \( KG = (V, E, \varphi, \psi) \), metaPathLength

**output:** A dictionary metapaths containing for metapaths\([u, v]\) all meta-paths between nodes \( u \) and \( v \)

**Function** computeMetaPaths(int metaPathLength)

for \( v \in V \) do
  computeMetaPaths\((v, v, \text{metaPathLength}, \text{empty metapath})\);
end

**Function** computeMetaPaths(current node \( v \), start node \( u \), int metaPathLength, Meta-path metapath)

if \( \text{metaPathLength} <= 0 \) then
  return;
end
metapath.append(\( \varphi(v) \)));
metapaths \([u, v]\).append(metapath);
adjacentNodes \( \left\{ x | (w, x) \in E \text{ or } (x, w) \in E \right\} \);
for \( y \in \text{adjacentNodes} \) do
  metapath.append(\( \psi(v, y) \)));
  computeMetaPaths\((y, u, \text{metaPathLength} - 1, \text{metapath})\)
end

The worst case runtime of this algorithm is \( \mathcal{O}(|V|^{|V|^{\text{length}}} = \mathcal{O}(|V|^{\text{length}+1}) \) for a fully connected graph. Luckily, knowledge graphs are in most cases not fully connected and the average case runtime is a more realistic approximation. The average case runtime is \( \mathcal{O}(|V| * \overline{\text{deg}}^{\text{length}} \) with the average node degree \( \overline{\text{deg}} \), if we assume that the degree is equally distributed over all nodes. This makes a big difference in knowledge graphs such as Wikidata because the average degree \( \overline{\text{deg}} \approx 5 \ll |V| \approx 4 \times 10^7 \).

The memory consumption of our algorithm is mainly determined by the number of meta-paths. The worst case number of meta-paths is \( \mathcal{O}((|\mathcal{A}|||\mathcal{R}||^{\text{length} - 1} |\mathcal{A}|) \), if the schema of the graph is fully connected. The average case number of meta-paths is roughly \( \mathcal{O}((\text{avg.nodetypes} * \text{avg.degree})^{\text{length} - 1} * \text{avg.nodetypes}) \) with \( \text{avg.nodetypes} \) being the average number of node types per node, if we assume that \( \text{avg.nodetypes} \) is equally distributed over all nodes. \( \text{avg.degree} \) is hereby the upper bound of the number of edge types for the edges connected with one node. The number of meta-paths scales with the number of node and edge types, which results in a high number of meta-paths in knowledge graphs.
As one can see, the algorithm has a high runtime complexity for calculating a huge number of meta-paths. One can compare our situation with the attempt to collect all text documents written at any time to accumulate all possible contexts of one word. With this comparison, it is clear that the complete enumeration of meta-paths is not needed for the embedding.

Following this finding, we can mine meta-paths probabilistically by skipping nodes and edges in the traversal. The result is equally to first calculating all meta-paths and then sampling from them with the exception that longer meta-paths are more rarely found by our algorithm. The reasons for this is that the probability of one specific path is \((1 - \text{edgeSkipProbability})^{\text{length}}\) and therefore gets smaller if we consider longer paths.

Algorithm 2 gets a knowledge graph \(KG = (V, E, \varphi, \psi)\) consisting of a graph \(G = (V, E)\) with node labeling function \(\varphi\) and edge labeling function \(\psi\) and \(\text{metaPathLength}\) specifying the maximum meta-path length as input like the deterministic Algorithm 1. Additional inputs are the \(\text{nodeSkipProbability}\) specifying the probability of skipping one node in the outer loop and the \(\text{edgeSkipProbability}\) specifying the probability of skipping one edge in the recursion. The addition in the probabilistic algorithm is that it skips nodes when it calls the function \(\text{probabilisticallyComputeMetaPaths}\) for each node in the graph.

The function \(\text{probabilisticallyComputeMetaPaths}\) gets the \(\text{metapath}\) up to this point, the start node \(u\), the current node \(v\) and \(\text{edgeSkipProbability}\) specifying the probability of skipping one edge as input. It only recursively calls itself if a random draw was successful and skips the edge otherwise. This algorithm produces the same results as performing random walks with a restart probability of \(\text{edgeSkipProbability}\), a restart probability of 1 if the random walk reaches length \(\text{length}\) and a uniformly distributed transition probability would. But due to the possible repeated traversal of the same edge, random walks are inefficient compared to our algorithm.

The embedding model for the modified algorithm does not change with the exceptions that the meta-path vocabulary \(MP\) gets \(\tilde{MP}_{p,q}\) of size \(|\tilde{MP}_{p,q}|\) and the context \(C_t\) of the meta-path with index \(t\) gets \(\tilde{C}_{t,p,q}\) with node skip probability \(p\) and edge skip probability of \(q\). We assume that the Meta-path vocabulary \(\tilde{MP}\) is roughly the same as \(MP\) because one meta-path occurs many times. Therefore, it is unlikely that we miss it completely.
Algorithm 2: Probabilistic Meta-Path Mining

**input**: $KG = (V, E, \varphi, \psi)$, \textit{metaPathLength}, \textit{nodeSkipProbability}, \textit{edgeSkipProbability}

**output**: A dictionary \textit{metapaths} containing for \textit{metapaths}[u, v] meta-paths between nodes $u$ and $v$

**Function** \textit{probabilisticallyComputeMetaPaths}(int \textit{metaPathLength}, float \textit{edgeSkipProbability}, float \textit{nodeSkipProbability})

\begin{algorithmic}
  \Function{probabilisticallyComputeMetaPaths}{current node $v$, start node $u$, int \textit{metaPathLength}, Meta-path \textit{metapath}, float \textit{edgeSkipProbability}}
  \If{$\textit{metaPathLength} < 0$}
  \State return;
  \EndIf
  \State \textit{metapath}.append($\varphi(v)$);
  \State \textit{metapaths}[u, v].append(\textit{metapath});
  \State adjacentNodes $\leftarrow \{x|(w, x) \in E \text{ or } (x, w) \in E\}$
  \For{$y \in$ adjacentNodes}
    \If{random()} $>$ \textit{edgeSkipProbability}
      \State \textit{metapath}.append($\psi(v, y)$);
      \State computeMetaPaths($y$, $u$, \textit{metaPathLength} − 1, \textit{metapath}, \textit{edgeSkipProbability})
    \EndIf
  \EndFor
\EndFunction
\end{algorithmic}
Neelakantan et al. [55] and Lin et al. [49] select a subset of relationship paths through sampling and pruning which is similar to the probabilistic meta-path mining. When executing our algorithm on a graph with a high number of node types, a higher `edgeSkipProbability` and lower `nodeSkipProbability` is preferable to start the mining from all node types even if it does not discover the whole neighborhood.

By not subsampling the graph in the beginning, we achieve an embedding of all node and edge types. Skipping edges and nodes results in a reduced but still big enough amount of training data. If we would first subsample the graph, we could calculate the full amount of training data for the embedding. However, this embedding would not contain all node and edge types and would therefore be only limited in its applicability.
4 Evaluation

In this section, we evaluate our embedding model by comparing it with baseline methods and showing the influence of different parameters.

We can not use standard datasets such as Freebase15k [15] and Freebase1M [15] (*not published*) to compare our method to previously published results. These datasets only include edge types and lack node types. This would not be a problem, if the edges would define a taxonomy. Unfortunately, the *type/object/type* relation [8] which defines the taxonomy of Freebase is not included in Freebase15k. Without the taxonomy, we can not define node types.

The other kind of dataset used in previous works are academic knowledge graphs such as DBLP. Generally speaking, they have a very small schema and for that reason only very few meta-paths. Our method is designed for rich schemata and we can not evaluate it meaningful with only very few node and edge types.

**Dataset** We use Wikidata [87] for our experiments because it is a constantly growing, freely available and large knowledge graph. Wikidata consists of entities which are either items or properties. Properties are used to link items together. Items are 'all the things in human knowledge, including topics, concepts, and objects'. Abstract concepts can be linked together with properties such as *part of*, *subclass of* and *is instance of* and objects with properties such as *material used*, *brand* and *has part*. Claims are statements about a feature of an item which consists of a property and a value. Wikidata can be transformed into a graph defining the items, properties and claims as nodes and the links between the nodes defined with properties as edges.

The Wikidata snapshot from 19th March 2018 used in the following experiments has roughly 45,770,000 entities and 237,950,000 claims. Claims do not carry useful information for embedding meta-paths because their values are for example coordinates, geographic shapes, quantities and URLs. Hence, we can exclude claims from our experiments.

There are no explicit node types in Wikidata, only a class hierarchy itself expressed as nodes linked together with *subclass of* properties. We use this class hierarchy as possible node types in the graph. We follow the *u - is instance of - v* relation of each node *u*, which is not in the class hierarchy, to assign the node label of node *v* to it. The class hierarchy forms a tree of height 40 and is very fine grained in the lower parts. We reduce the tree to a height of *n* by traversing it from the

[8] https://www.wikidata.org/wiki/Help:Items
root and adding the class labels of the higher nodes to the lower ones up to depth $n$. All levels from there to the leaves get the class labels from above. This causes an abstraction of the fine-grained classes and enables us to learn an embedding of each class and its superclasses simultaneously.

### 4.1 Link Prediction in Knowledge Graphs

We use the problem of link prediction to evaluate the quality of our embedding. In the following, we evaluate two of our three proposed feature definitions for nodes and edges from Sections 3.2.1, 3.2.2 and 3.2.3.

We use the Wikidata version from the 19th March 2018 (time step $t_0$) and 2nd April 2018 (time step $t_1$) for our experiments and transform them as described above. We set the height of the class hierarchy to 3 and mine meta-paths of length 5 with a $\text{nodeSkipProbability}$ of 0.9999 and an $\text{edgeSkipProbability}$ of 0.99 to get a reasonable amount of data. An incomplete run with $\text{nodeSkipProbability}$ of 0 produces 3TB in two days runtime.

Between time step $t_0$ and time step $t_1$, 3,047,829 new edges were added to Wikidata. 2,257,380 of these edges contain at least one node which was added to Wikidata in $t_1$. Hence, 790,449 edges are left for which we can calculate a representation solely based on $t_0$ and therefore use for our link prediction experiment with the meta-path-based node representation. Using the different representations, we train a logistic regression model ten times for each measurement and report the average in the following experiments. Generally, 50% of the new edges are used for training and 50% are used for testing.

Our experiments are based on the argumentation of Davis et al. [19] that different links have different formation mechanisms. If these formation mechanisms correlate with the different dimensions of the embedding, the model should be able to distinguish the mechanisms. The correlation could be caused by the fact that the different dimensions represent concepts such as the domains which are determining the formation mechanisms.

Our first finding is that logistic regression does not significantly profit from more than 0.5% of the data as can be seen in Figure[1]. This finding allows us to perform the following experiments on a subset of all new edges.
4 Evaluation

![Graph showing the macro F1 score for different percentages of new edges.](image)

Figure 1: Showing the macro F1 score for different percentages of new edges.

| emb. dim. | 16 | 32 | 64 | 128 | 256 |
|-----------|----|----|----|-----|-----|
| F1 score  | 0.67 | 0.67 | 0.73 | 0.72 | 0.72 |

Table 2: Macro F1 scores for the link prediction on 1% of Wikidata using different embedding sizes.

4.1.1 Node type-based Node Embedding

The node type-based node embedding from Section 3.2.3 serves as a baseline to evaluate our approach. The experiments in Table 2 show that we produce a good embedding regarding the node and edge types. This is an indicator that we also embed the meta-paths sensibly because they are the combination of these types and define the objective function for the embedding. Furthermore, our approach is insensitive regarding the number of dimensions and can produce a good embedding with a relatively low number of dimensions. The best performance in both node embeddings is achieved with a dimensionality of 64. The invariable performance could also be a sign that the logistic regression is not expressive enough for modeling more complex relations in the embeddings with a high number of dimensions. To check this, we should repeat these experiments with a more expressive model and compare the performance.

Additionally, the experiments in Table 3 show that the embedding is insensitive with one exception to the vector operator we use to combine two node embeddings to an edge embedding.
4.1 Link Prediction in Knowledge Graphs

|                       | Average | Concat | Hadamard | Weighted L1 | Weighted L2 |
|-----------------------|---------|--------|----------|-------------|-------------|
|                       | 0.74    | 0.740  | 0.72     | 0.48        | 0.74        |

Table 3: Macro F1 scores for the link prediction on 1% of Wikidata using different vector operators to combine two node embeddings to an edge embedding.

| emb. dim. | 128 | 256 | 512 | 1024 |
|-----------|-----|-----|-----|------|
| F1 score  | 0.58| 0.57| 0.58| 0.58 |

Table 4: Macro F1 scores for the link prediction using meta-path-based node embeddings on 1% of Wikidata with different embedding dimensions.

4.1.2 Meta-path-based Node Embedding

For the meta-path-based node embedding, we have to exclude new nodes and therefore edges involving a new node from the link prediction. This is based on the fact that we can not mine meta-paths for these nodes in the graph at time step $t_0$. Mining meta-paths starting in one node of the 790449 new edges with an edgeSkipProbability of 0.999 yields meta-paths between 1 543 422 pairs of nodes. If we assume that all the nodes in these edges are distinct, the mean number of meta-path sets for one node is 1. A set of meta-paths is defined as all the meta-paths which connect two nodes. In practice, we have 356 216 instead of the possible 1 580 898 distinct nodes. Therefore, we have on average 4.3 sets of meta-paths for one node. Because we ignore the direction, we can also use the meta-paths ending in this node.

We can speed up the mining of meta-paths by introducing a stop criterion based on the number of meta-paths the algorithm has found for one node because we don’t need many meta-paths to represent one node. In the following experiment, this parameter is set to 10 meta-paths per node. If we do not find any meta-paths for a node, we use the zero vector to represent it. For the task of link prediction, we have to combine the embeddings of the two nodes of an edge to get the edge embedding. With the use of the zero vector, we can not use multiplicative vector operators such as the hadamard product. Therefore, we average the two node embeddings to derive the edge embedding.

The results in Table 4 show that the current configuration of the node embedding based on meta-paths is significantly worse than the node type-based one. The experiments in Section 4.1.2 show that the embeddings learn a sensible representation for at least the node and edge types. However, the meta-path-based node embedding does not use this information for a good representation of the nodes.
## Evaluation

| emb. dim. | 16 | 32 | 64 | 128 | 256 |
|-----------|----|----|----|-----|-----|
| F1 score  | 0.56 | 0.57 | 0.59 | 0.57 | 0.58 |

Table 5: Macro F1 scores for the link prediction using meta-path-based node embeddings with the minimal size of the n-grams set to 1. The experiments were conducted on 1% of Wikidata with different embedding dimensions.

The reason for this could be that the meta-paths are not adequately captured in the embedding. This is unlikely because it captures the node and edge types despite the fact that the objective only concerns the meta-paths. It is more likely that we do not represent the nodes well enough in the way we combine the meta-path embedding to a node embedding. One problem could be that many nodes have very many meta-paths and an average of all these meta-paths is not very meaningful. One the other side, picking some meta-paths randomly to reduce the number probably also does not capture the node well. One possible approach to solve this issue could be to only use the most frequent meta-paths for the node embedding.

When comparing the experiments in Table 4 and 5, we see that the inclusion of direct node and edge type embeddings neither improves nor impairs the performance. Therefore, it is advisable to include these embeddings to be able to calculate a node type-based node embedding using the meta-path embedding.

### 4.1.3 Meta-path-based Edge Embedding

As in Section 4.1.2, we have to exclude new nodes from the training set and learn our prediction model on the reduced number of training samples. With an `nodeSkipProbability` of 0.999 resulting in 700 edges and an `edge.SkipProbability` of 0, only for 3 edges meta-paths of length 3 are found. We should further investigate if the meta-paths are really missing in $t_0$ or if it is a problem with the way we mine them. The problem is most probably caused by the high probability of skipping edges. To solve this issue, we should not search them in a breadth-first manner and instead direct the search by calculating the shortest path between these nodes.

If we make the assumption that the direction of the edges is not important as we did in our algorithm, the search can be modeled as an all-pairs-shortest-path problem on undirected and unweighted graphs. This problem can be solved with Seidel’s algorithm \[67\] in $O(|V|^\omega \log |V|)$ where $O(n^\omega)$ is the complexity of a $n \times n$ matrix multiplication. The current upper bound of $\omega$ is roughly 2.373 [40].

When computing the shortest path, we get only one meta-path between the two nodes under the premise that the shortest path exists. If one meta-path is not enough to represent the edge, we could formulate the search as the k shortest
4.1 Link Prediction in Knowledge Graphs

Table 6: Macro F1 scores for link prediction on Wikidata using differing amounts of new edges. We compare DeepWalk, VERSE, node2vec and our method based on the node type embedding. The vector operator is hadamard. The node type embedding is calculated on full wikidata. "-" marks that the method can not handle the number of nodes.

| Percentage | Verse [85] | Deepwalk [64] | node2vec [27] | Node types |
|------------|------------|---------------|---------------|-------------|
| 1%         | 0.61       | 0.64          | -             | 0.72        |
| 2.5%       | 0.74       | -             | -             | 0.59        |
| 5%         | 0.83       | -             | -             | 0.59        |
| 100%       | -          | -             | -             | 0.74        |

paths problem [23]. Eppstein [23] proposes an algorithm for k shortest paths from one node to all others in $O(|E| + |V|\log|V| + k|V|)$. This algorithm can be restarted from every node to solve the all-pairs-k-shortest-path problem in $O(|V|(|E| + |V|\log|V| + k|V|)) = O(|V|^2 + |V|^2\log|V| + k|V|^2)$.

Further experiments should be done to determine the right size of the context window and to what extent the embedding should be regularized by excluding too frequent and infrequent meta-paths/n-grams.

4.1.4 Comparison with Node Embedding Methods

The used implementations of DeepWalk[^3] node2vec[^4] and VERSE[^5] can not handle the complete Wikidata dataset because the required memory exceeds the 1TB RAM of our server. We are using the same 1%, 2.5% and 5% of Wikidata for the following experiments with VERSE and DeepWalk. As one can see in Table 6 DeepWalk can not handle more than 1% and VERSE 5% of Wikidata. Node2vec can not even handle 1% of it.

The following experiments are on denser subsamples than the complete Wikidata dataset because we sample from the edges and therefore have a bias for nodes with a high degree. We would expect a better performance of VERSE and DeepWalk on these subsamples as on the real dataset because they get more structural information. Our method would profit from a subsampling of the nodes because a node with many neighbors also has many meta-paths which does lead to a very unspecific representation. The increasing performance of VERSE in Table 6 can be explained by the fact that it embeds more nodes with a similar structure and

[^3]: https://github.com/xgfs/deepwalk-c
[^4]: https://github.com/xgfs/node2vec-c
[^5]: https://github.com/xgfs/verse
for this reason the regression model gets more training data with the same representation. The embeddings of our method are trained on the full graph and the regression model gets only the corresponding subsets. Our method would not profit from training it on these smaller graphs because we need multiple contexts for a meta-path to embed it sensibly. In comparison, VERSE and DeepWalk can specialize if they are confronted with a smaller subgraph. It is not completely clear why our method performs considerably worse on 2.5% and 5% in comparison with 1% and 100% of Wikidata. One reason could be that we sample two subsets which are not representative for the full data or that our method can not deal with the way we subsample the graph.

4.2 Future Experiments

After our first experimental evaluation, further experiments should be done to compare our method with other approaches, evaluate it on other tasks, validate the generalization on other datasets and test the sensitivity of parameters we did not check.

We expect that our method generalizes to other datasets well because we did not make any assumptions specific for Wikidata. The depth of the class hierarchy is a parameter to which we would attribute a high influence on our method but did not check yet. If the depth is too high, the embedding model does not get enough signal for infrequent node types. If the depth is too low, only very high level classes are included in the meta-paths which are not expressive enough for the down stream task. The nodeSkipProbability and edgeSkipProbability determine if the training data covers all edge and node types in the graph and if the embedding model gets a representative sample of the graph. An open question is the influence of the amount of training data. Additional models to compare with are the translational approaches. Using our node embeddings, we can perform more classical node embedding experiments such as node clustering, node classification and graph reconstruction.

4.2.1 Does the Embedding Capture the Concepts Which the Meta-paths Represent?

With the following experiment we could check if the embedding has captured the concepts which the meta-paths represent. The underlying assumption is that similar concepts occur together. For example, movie-related concepts occur between two specific actors but not together with transportation-related concepts. To verify the similarity of co-occurring concepts, we predict the presence of meta-paths
instead of simple edges between two nodes. For this experiment, we first have to mine all meta-paths between some nodes, sample one not existing meta-path for each existing one and then train a predictor. The features for this predictor are all meta-paths between two nodes expect of one combined. The excluded meta-path is used as label. If the model succeeds in predicting co-occurring concepts, we have evidence that the embedding captures the concepts. The critical part of this experiment is that the computation of all meta-paths between some nodes is computationally very expensive. We should first investigate if it is sufficient to probabilistically mine meta-paths between the two nodes. The probabilistic version of the experiment is only valid if the probability of incorrectly sampling a meta-path as a negative example is low enough.

Correlating meta-paths A similar test can be performed by first searching for the most correlating meta-paths and then comparing their embeddings. Correlation of meta-paths means that meta-paths are occurring together between pairs of nodes. For the same reasons as in the above experiment, the embeddings should be similar. Therefore, we can compare the quality of different embeddings by summing up a similarity measure such as cosine similarity of the embedding of the top n most correlating meta-paths.

4.2.2 Link Type Prediction in Knowledge Graphs

The extension of the link prediction experiment is the prediction if a link will form and which type it will have. Sun et al. [79] introduce this problem as relationship prediction. This could be performed by a two stage process where we first predict the link forming and afterwards the type for the formed links. One can reuse the predictor from Section 4.1 with this structure. Another option would be to model "no link" as an extra edge type and then directly learn a predictor for the extended edge types. We would expect a significantly better prediction performance of our meta-path-based approach in comparison with methods which only use the structure of the graph. An even more complicated version of this experiment is to predict when a link will form [79].
4 Evaluation

4.2.3 Knowledge Graph Completion

Our technique can also be used for knowledge graph completion. In this case, the meta-path-based edge embeddings should not suffer from the problem that nodes which are part of new edges are only sparsely connected by meta-paths. Therefore, this task would be a good experiment to compare edge features based on node and edge embeddings.
5 Implementation Details

In this section, we shortly describe and evaluate the pipeline of our experiments.

The graphs were imported into neo4j instances for a unified access and manipulation. We used the wikidata-neo4j-importer to import Wikidata JSON dumps into neo4j. This import takes up to one week and should be optimized for future experiments.

The conversion of the class hierarchy and the assignment of node types to the nodes as described in Section are implemented as procedures in neo4j. The mining of meta-paths as described in Section with Algorithms and is also implemented as a procedure in neo4j. This calculation can be scaled over a cluster without synchronization overhead because each computing node can be limited to mine the meta-paths in a specific range of start nodes. The computation of meta-paths on one computing node is even faster than the disks of the storage system can save them.

Afterwards, we combine the meta-paths between two nodes to form sentences as described in Section and train the embeddings using fastText. Simultaneously, we search with neo4j cypher queries for new edges between and and exclude edges which new nodes. We perform the meta-path-based link prediction experiments using our experimentation framework. For a detailed description, please see Rückin [65].

1. https://github.com/findie/wikidata-neo4j-importer
2. https://github.com/Baschdl/neo4j-graph-algorithms/tree/multiTypesConversion
3. https://github.com/facebookresearch/fastText
4. https://github.com/Baschdl/metapath-embedding
5. https://github.com/Baschdl/bachelor-thesis-experiments/tree/metapath_embedding
6 Conclusion

In this work, we introduced the first embedding model for meta-paths. This model is especially designed to deal with the high redundancy and high amount of meta-paths in big knowledge graphs. Furthermore, it allows the training of machine learning models on the semantic properties of meta-paths. Using the meta-path embedding model, we defined new node and edge type embeddings. Additionally, we proposed new general vector representations for edges and nodes based on meta-paths.

We found problems in the first experiments regarding the presence of meta-paths between nodes which will be part of an edge in the future. Here, we have to experiment with a meta-path mining approach using shortest path algorithms to solve these problems or prove that our assumption regarding the connectivity was wrong. Especially our edge embeddings look promising for tasks such as link prediction. These tasks concern edges but the current methods only use node embeddings to calculate features for them and no edge-specific features. When dealing with real world knowledge graphs, we can not avoid to use subsampling with current methods. But our method performs it in a way which does not hurt the applicability of our embedding in contrast to the experiments in most other works. In our experiments, we found evidence that our method produces sensible embeddings but we have to make further experiments to work on current problems and compare it to the group of translational approaches.

Further investigation should be done concerning the influence of the data and parameter settings. We further have to evaluate how much data our method needs and how we can adjust the collection process to it. One could also imagine to learn a meta-path embedding by only learning node type and edge type embeddings and combining them to a meta-path embedding afterwards. Building up on our embedding model, one could investigate if there is a better representation of parts of a meta-path than n-grams. Another way of improving the model could be to use the structure of the class hierarchy and the property that nodes have multiple labels more directly in the embedding process.
7 Acknowledgements

I thank my supervisors Davide and Prof. Emmanuel Müller for their commitment to the bachelor project and their support, our project partners for providing the initial problem and continuous support, my bachelor project team for the work together, especially Julius for jointly implementing the experiment framework and discussing specific aspects of my thesis and Freya for asking all the critical questions, and my proof readers, especially Samuel for discussing my thesis so thoroughly.
References

[1] L. A. Adamic and E. Adar. Friends and neighbors on the web. Social networks, 25(3):211–230, 2003.

[2] A. Ahmed, N. Shervashidze, S. Narayanamurthy, V. Josifovski, and A. J. Smola. Distributed large-scale natural graph factorization. In Proceedings of the 22nd international conference on World Wide Web, pages 37–48. ACM, 2013.

[3] L. Akoglu, H. Tong, and D. Koutra. Graph based anomaly detection and description: a survey. Data mining and knowledge discovery, 29(3):626–688, 2015.

[4] L. A. N. Amaral. A truer measure of our ignorance. Proceedings of the National Academy of Sciences, 105(19):6795–6796, 2008.

[5] S. Auer, C. Bizer, G. Kobilarov, J. Lehmann, R. Cyganiak, and Z. Ives. Dbpedia: A nucleus for a web of open data. In The semantic web, pages 722–735. Springer, 2007.

[6] A.-L. Barabási, H. Jeong, Z. Néda, E. Ravasz, A. Schubert, and T. Vicsek. Evolution of the social network of scientific collaborations. Physica A: Statistical mechanics and its applications, 311(3-4):590–614, 2002.

[7] M. Baroni and A. Lenci. Distributional memory: A general framework for corpus-based semantics. Computational Linguistics, 36(4):673–721, 2010.

[8] H. Bast, F. Bäurle, B. Buchhold, and E. Haußmann. Easy access to the freebase dataset. In Proceedings of the 23rd International Conference on World Wide Web, pages 95–98. ACM, 2014.

[9] F. Behrens, S. Bischoff, P. Ladenburger, J. Rückin, L. Seidel, F. Stolp, M. Vaichenker, A. Ziegler, D. Mottin, F. Aghaei, et al. Metaexp: Interactive explanation and exploration of large knowledge graphs. In Companion of the The Web Conference 2018 on The Web Conference 2018, pages 199–202. International World Wide Web Conferences Steering Committee, 2018.

[10] D. M. Blei, A. Y. Ng, and M. I. Jordan. Latent dirichlet allocation. Journal of machine Learning research, 3(Jan):993–1022, 2003.

[11] R. Blumberg and S. Atre. The problem with unstructured data. Dm Review, 13(42-49):62, 2003.
[12] P. Bojanowski, E. Grave, A. Joulin, and T. Mikolov. Enriching word vectors with subword information. *Transactions of the Association for Computational Linguistics*, 5:135–146, 2017.

[13] K. Bollacker, C. Evans, P. Paritosh, T. Sturge, and J. Taylor. Freebase: a collaboratively created graph database for structuring human knowledge. In *Proceedings of the 2008 ACM SIGMOD international conference on Management of data*, pages 1247–1250. AcM, 2008.

[14] A. Bordes, J. Weston, R. Collobert, Y. Bengio, et al. Learning structured embeddings of knowledge bases. In *AAAI*, volume 6, page 6, 2011.

[15] A. Bordes, N. Usunier, A. Garcia-Duran, J. Weston, and O. Yakhnenko. Translating embeddings for modeling multi-relational data. In *Advances in neural information processing systems*, pages 2787–2795, 2013.

[16] A. Bordes, N. Usunier, J. Weston, and O. Yakhnenko. Translating Embeddings for Modeling Multi-Relational Data. *Advances in NIPS*, 26:2787–2795, 2013. ISSN 10495258. doi: 10.1007/s13398-014-0173-7.

[17] A. Bordes, X. Glorot, J. Weston, and Y. Bengio. A semantic matching energy function for learning with multi-relational data. *Machine Learning*, 94(2):233–259, 2014.

[18] S. Cao, W. Lu, and Q. Xu. Grarep: Learning graph representations with global structural information. In *Proceedings of the 24th ACM International on Conference on Information and Knowledge Management*, pages 891–900. ACM, 2015.

[19] D. Davis, R. Lichtenwalter, and N. V. Chawla. Multi-relational link prediction in heterogeneous information networks. In *Advances in Social Networks Analysis and Mining (ASONAM), 2011 International Conference on*, pages 281–288. IEEE, 2011.

[20] S. Deerwester, S. T. Dumais, G. W. Furnas, T. K. Landauer, and R. Harshman. Indexing by latent semantic analysis. *Journal of the American society for information science*, 41(6):391–407, 1990.

[21] T. Dettmers, P. Minervini, P. Stenetorp, and S. Riedel. Convolutional 2d knowledge graph embeddings. *arXiv preprint arXiv:1707.01476*, 2017.

[22] Y. Dong, N. V. Chawla, and A. Swami. metapath2vec: Scalable representation learning for heterogeneous networks. In *Proceedings of the 23rd ACM
References

SIGKDD International Conference on Knowledge Discovery and Data Mining, pages 135–144. ACM, 2017.

[23] D. Eppstein. Finding the k shortest paths. SIAM Journal on computing, 28 (2):652–673, 1998.

[24] A. Garcia-Duran, A. Bordes, N. Usunier, and Y. Grandvalet. Combining Two And Three-Way Embeddings Models for Link Prediction in Knowledge Bases. 55:715–742, 2015. doi: 10.1613/jair.5013.

[25] M. Gardner and T. Mitchell. Efficient and expressive knowledge base completion using subgraph feature extraction. In Proceedings of the 2015 Conference on Empirical Methods in Natural Language Processing, pages 1488–1498, 2015.

[26] A. Graves. Generating sequences with recurrent neural networks. arXiv preprint arXiv:1308.0850, 2013.

[27] A. Grover and J. Leskovec. node2vec: Scalable feature learning for networks. In Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining, pages 855–864. ACM, 2016.

[28] S. Guo, Q. Wang, B. Wang, L. Wang, and L. Guo. Semantically smooth knowledge graph embedding. In Proceedings of the 53rd Annual Meeting of the Association for Computational Linguistics and the 7th International Joint Conference on Natural Language Processing (Volume 1: Long Papers), volume 1, pages 84–94, 2015.

[29] M. Gupta, V. Varma, et al. Doc2sent2vec: A novel two-phase approach for learning document representation. In Proceedings of the 39th International ACM SIGIR conference on Research and Development in Information Retrieval, pages 809–812. ACM, 2016.

[30] K. Guu, J. Miller, and P. Liang. Traversing knowledge graphs in vector space. In Proceedings of the 2015 Conference on Empirical Methods in Natural Language Processing, pages 318–327, 2015.

[31] Z. S. Harris. Distributional structure. Word, 10(2-3):146–162, 1954.

[32] J. Hoffart, F. M. Suchanek, K. Berberich, and G. Weikum. Yago2: A spatially and temporally enhanced knowledge base from wikipedia. Artificial Intelligence, 194:28–61, 2013.

[33] T. Hofmann. Probabilistic latent semantic indexing. In Proceedings of the
References

22nd annual international ACM SIGIR conference on Research and development in information retrieval, pages 50–57. ACM, 1999.

[34] Z. Huang, Y. Zheng, R. Cheng, Y. Sun, N. Mamoulis, and X. Li. Meta structure: Computing relevance in large heterogeneous information networks. In Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pages 1595–1604. ACM, 2016.

[35] L. Katz. A new status index derived from sociometric analysis. Psychometrika, 18(1):39–43, 1953.

[36] Y. Kim, Y. Jernite, D. Sontag, and A. M. Rush. Character-aware neural language models. In AAAI, pages 2741–2749, 2016.

[37] X. Kong, P. S. Yu, Y. Ding, and D. J. Wild. Meta path-based collective classification in heterogeneous information networks. In Proceedings of the 21st ACM international conference on Information and knowledge management, pages 1567–1571. ACM, 2012.

[38] N. Lao and W. W. Cohen. Relational retrieval using a combination of path-constrained random walks. Machine learning, 81(1):53–67, 2010.

[39] Q. Le and T. Mikolov. Distributed representations of sentences and documents. In International Conference on Machine Learning, pages 1188–1196, 2014.

[40] F. Le Gall. Powers of tensors and fast matrix multiplication. In Proceedings of the 39th international symposium on symbolic and algebraic computation, pages 296–303. ACM, 2014.

[41] D. Lenat and E. Feigenbaum. On the thresholds of knowledge. Foundations of Artificial Intelligence, MIT Press, Cambridge, MA, pages 185–250, 1992.

[42] O. Levy and Y. Goldberg. Neural word embedding as implicit matrix factorization. In Advances in neural information processing systems, pages 2177–2185, 2014.

[43] D. Liben-Nowell and J. Kleinberg. The link-prediction problem for social networks. Journal of the American society for information science and technology, 58(7):1019–1031, 2007.

[44] R. N. Lichtenwalter, J. T. Lussier, and N. V. Chawla. New perspectives and methods in link prediction. In Proceedings of the 16th ACM SIGKDD
References

[45] H. Lin, Y. Liu, W. Wang, Y. Yue, and Z. Lin. Learning Entity and Relation Embeddings for Knowledge Resolution. *Procedia Computer Science*, 108:345–354, 2017. ISSN 18770509. doi: 10.1016/j.procs.2017.05.045.

[46] Y. Lin, Z. Liu, H. Luan, M. Sun, S. Rao, and S. Liu. Modeling relation paths for representation learning of knowledge bases. In *Proceedings of the 2015 Conference on Empirical Methods in Natural Language Processing*, pages 705–714, 2015.

[47] X. Liu, Y. Yu, C. Guo, and Y. Sun. Meta-path-based ranking with pseudo relevance feedback on heterogeneous graph for citation recommendation. In *Proceedings of the 23rd acm international conference on conference on information and knowledge management*, pages 121–130. ACM, 2014.

[48] L. Lü and T. Zhou. Link prediction in complex networks: A survey. *Physica A: statistical mechanics and its applications*, 390(6):1150–1170, 2011.

[49] Y. Luo, Q. Wang, B. Wang, and L. Guo. Context-dependent knowledge graph embedding. In *Proceedings of the 2015 Conference on Empirical Methods in Natural Language Processing*, pages 1656–1661, 2015.

[50] C. Meng, R. Cheng, S. Maniu, P. Senellart, and W. Zhang. Discovering meta-paths in large heterogeneous information networks. In *WWW*, pages 754–764, 2015.

[51] T. Mikolov, I. Sutskever, A. Deoras, H.-S. Le, and S. Kombrink. Subword language modeling with neural networks.

[52] T. Mikolov, K. Chen, G. Corrado, and J. Dean. Efficient estimation of word representations in vector space. *arXiv preprint arXiv:1301.3781*, 2013.

[53] T. Mikolov, I. Sutskever, K. Chen, G. S. Corrado, and J. Dean. Distributed representations of words and phrases and their compositionality. In *Advances in neural information processing systems*, pages 3111–3119, 2013.

[54] B. Murphy, P. Talukdar, and T. Mitchell. Learning effective and interpretable semantic models using non-negative sparse embedding. *Proceedings of COLING 2012*, pages 1933–1950, 2012.

[55] A. Neelakantan, B. Roth, and A. McCallum. Compositional vector space models for knowledge base completion. In *Proceedings of the 53rd Annual
References

Meeting of the Association for Computational Linguistics and the 7th International Joint Conference on Natural Language Processing (Volume 1: Long Papers), volume 1, pages 156–166, 2015.

[56] M. E. Newman. Clustering and preferential attachment in growing networks. Physical review E, 64(2):025102, 2001.

[57] D. Q. Nguyen. An overview of embedding models of entities and relationships for knowledge base completion. arXiv preprint arXiv:1703.08098, 2017.

[58] D. Q. Nguyen, K. Sirts, L. Qu, and M. Johnson. Neighborhood mixture model for knowledge base completion. CoNLL 2016, page 40, 2016.

[59] D. Q. Nguyen, T. D. Nguyen, D. Q. Nguyen, and D. Phung. A novel embedding model for knowledge base completion based on convolutional neural network. In Proceedings of the 2018 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 2 (Short Papers), volume 2, pages 327–333, 2018.

[60] M. Nickel, K. Murphy, V. Tresp, and E. Gabrilovich. A review of relational machine learning for knowledge graphs. Proceedings of the IEEE, 104(1):11–33, 2016.

[61] M. Nickel, L. Rosasco, T. A. Poggio, et al. Holographic embeddings of knowledge graphs. In AAAI, volume 2, pages 3–2, 2016.

[62] M. Ou, P. Cui, J. Pei, Z. Zhang, and W. Zhu. Asymmetric transitivity preserving graph embedding. In Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining, pages 1105–1114. ACM, 2016.

[63] J. Pennington, R. Socher, and C. Manning. Glove: Global vectors for word representation. In Proceedings of the 2014 conference on empirical methods in natural language processing (EMNLP), pages 1532–1543, 2014.

[64] B. Perozzi, R. Al-Rfou, and S. Skiena. Deepwalk: Online learning of social representations. In Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining, pages 701–710. ACM, 2014.

[65] J. Rückin. Similarity explanation and exploration in a heterogeneous information network, 2018.

[66] A. Salle, M. Idiart, and A. Villavicencio. Matrix factorization using window
sampling and negative sampling for improved word representations. arXiv preprint arXiv:1606.00819, 2016.

[67] R. Seidel. On the all-pairs-shortest-path problem in unweighted undirected graphs. Journal of computer and system sciences, 51(3):400–403, 1995.

[68] C. Shi, X. Kong, P. S. Yu, S. Xie, and B. Wu. Relevance search in heterogeneous networks. In Proceedings of the 15th International Conference on Extending Database Technology, pages 180–191. ACM, 2012.

[69] C. Shi, X. Kong, Y. Huang, S. Y. Philip, and B. Wu. Hetesim: A general framework for relevance measure in heterogeneous networks. IEEE Trans. Knowl. Data Eng., 26(10):2479–2492, 2014.

[70] C. Shi, Y. Li, J. Zhang, Y. Sun, and S. Y. Philip. A survey of heterogeneous information network analysis. IEEE Transactions on Knowledge and Data Engineering, 29(1):17–37, 2017.

[71] R. Socher, D. Chen, C. D. Manning, and A. Ng. Reasoning with neural tensor networks for knowledge base completion. In Advances in neural information processing systems, pages 926–934, 2013.

[72] M. P. Stumpf, T. Thorne, E. de Silva, R. Stewart, H. J. An, M. Lappe, and C. Wiuf. Estimating the size of the human interactome. Proceedings of the National Academy of Sciences, 105(19):6959–6964, 2008.

[73] F. M. Suchanek, G. Kasneci, and G. Weikum. Yago: a core of semantic knowledge. In Proceedings of the 16th international conference on World Wide Web, pages 697–706. ACM, 2007.

[74] Y. Sun and J. Han. Mining heterogeneous information networks: principles and methodologies. Synthesis Lectures on Data Mining and Knowledge Discovery, 3(2):1–159, 2012.

[75] Y. Sun and J. Han. Mining heterogeneous information networks: a structural analysis approach. ACM SIGKDD Explorations Newsletter, 14(2):20–28, 2013.

[76] Y. Sun, Y. Yu, and J. Han. Ranking-based clustering of heterogeneous information networks with star network schema. In Proceedings of the 15th ACM SIGKDD international conference on Knowledge discovery and data mining, pages 797–806. ACM, 2009.

[77] Y. Sun, R. Barber, M. Gupta, C. C. Aggarwal, and J. Han. Co-author rela-
[78] Y. Sun, J. Han, X. Yan, P. S. Yu, and T. Wu. Pathsim: Meta path-based top-k similarity search in heterogeneous information networks. *PVLDB*, 4(11):992–1003, 2011.

[79] Y. Sun, J. Han, C. C. Aggarwal, and N. V. Chawla. When will it happen?: relationship prediction in heterogeneous information networks. In *Proceedings of the fifth ACM international conference on Web search and data mining*, pages 663–672. ACM, 2012.

[80] Y. Sun, B. Norick, J. Han, X. Yan, P. S. Yu, and X. Yu. Pathselclus: Integrating meta-path selection with user-guided object clustering in heterogeneous information networks. *ACM Transactions on Knowledge Discovery from Data (TKDD)*, 7(3):11, 2013.

[81] I. Sutskever, J. Martens, and G. E. Hinton. Generating text with recurrent neural networks. In *Proceedings of the 28th International Conference on Machine Learning (ICML-11)*, pages 1017–1024, 2011.

[82] J. Tang, M. Qu, M. Wang, M. Zhang, J. Yan, and Q. Mei. Line: Large-scale information network embedding. In *Proceedings of the 24th International Conference on World Wide Web*, pages 1067–1077. International World Wide Web Conferences Steering Committee, 2015.

[83] K. Toutanova and D. Chen. Observed versus latent features for knowledge base and text inference. In *Proceedings of the 3rd Workshop on Continuous Vector Space Models and their Compositionality*, pages 57–66, 2015.

[84] K. Toutanova, V. Lin, W.-t. Yih, H. Poon, and C. Quirk. Compositional learning of embeddings for relation paths in knowledge base and text. In *Proceedings of the 54th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, volume 1, pages 1434–1444, 2016.

[85] A. Tsitsulin, D. Mottin, P. Karras, and E. Müller. Verse: Versatile graph embeddings from similarity measures. In *Proceedings of the 2018 World Wide Web Conference on World Wide Web*, pages 539–548. International World Wide Web Conferences Steering Committee, 2018.

[86] P. D. Turney and P. Pantel. From frequency to meaning: Vector space models of semantics. *Journal of artificial intelligence research*, 37:141–188, 2010.
[87] D. Vrandečić and M. Krötzsch. Wikidata: a free collaborative knowledgebase. Communications of the ACM, 57(10):78–85, 2014.

[88] Q. Wang, J. Liu, Y. Luo, B. Wang, and C.-Y. Lin. Knowledge base completion via coupled path ranking. In Proceedings of the 54th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), volume 1, pages 1308–1318, 2016.

[89] Q. Wang, Z. Mao, B. Wang, and L. Guo. Knowledge graph embedding: A survey of approaches and applications. IEEE Transactions on Knowledge and Data Engineering, 29(12):2724–2743, 2017.

[90] Z. Wang, J. Zhang, J. Feng, and Z. Chen. Knowledge Graph Embedding by Translating on Hyperplanes. AAAI Conference on Artificial Intelligence, pages 1112–1119, 2014.

[91] R. Xie, Z. Liu, and M. Sun. Representation learning of knowledge graphs with hierarchical types. In IJCAI, pages 2965–2971, 2016.

[92] X. Yu, Q. Gu, M. Zhou, and J. Han. Citation prediction in heterogeneous bibliographic networks. In Proceedings of the 2012 SIAM International Conference on Data Mining, pages 1119–1130. SIAM, 2012.

[93] X. Yu, Y. Sun, B. Norick, T. Mao, and J. Han. User guided entity similarity search using meta-path selection in heterogeneous information networks. In Proceedings of the 21st ACM international conference on Information and knowledge management, pages 2025–2029. Acm, 2012.

[94] J. Zhang, P. S. Yu, and Z.-H. Zhou. Meta-path based multi-network collective link prediction. In Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining, pages 1286–1295. ACM, 2014.

[95] A. Ziegler. Active learning with curriculum on knowledge graphs, 2018.
In dieser Arbeit untersuchen wir das Lernen von Merkmalen auf heterogenen Wissensgraphen. Diese Merkmale können für Aufgaben wie die Vorhersage von Verbindungen, Klassifikation und Clustering verwendet werden. Wissensgraphen bieten eine reichhaltige Semantik, die in den Kanten- und Knotentypen codiert ist. Meta-Pfade bestehen aus diesen Typen und stellen eine Abstraktion von Pfaden im Graphen dar.

Bisher können Meta-Pfade nur als kategorische Merkmale mit hoher Redundanz verwendet werden. Wir stellen einen Ansatz zum Lernen von semantischen Präsentationen von Meta-Pfaden vor. Aktuelle Methoden können nur Präsentation für Knoten und Kantentypen lernen. Unser Ansatz benutzt ein erweitertes Skipgram-Modell um, trotz hoher Redundanz und Anzahl, Merkmale für Meta-Pfade zu lernen. Wir evaluieren unserer Methode mit der Vorhersage von Verbindungen auf Wikidata. Diese Experimente zeigen, dass wir eine sinnvolle Präsentation lernen. Allerdings müssen wir die Merkmale für die Vorhersage von Verbindungen verbessern und weitere Experimente durchführen.
Selbstständigkeitserklärung

Hiermit erkläre ich, die vorliegende Arbeit selbstständig angefertigt, nicht anderweitig zu Prüfungszwecken vorgelegt und keine anderen als die angegebenen Hilfsmittel verwendet zu haben. Sämtliche wissentlich verwendete Textausschnitte, Zitate oder Inhalte anderer Verfasser wurden ausdrücklich als solche gekennzeichnet.

Potsdam, den 30. Juli 2018

________________________________________
Sebastian Bischoff