DOLORES: Deep Contextualized Knowledge Graph Embeddings

Haoyu Wang¹, Vivek Kulkarni², William Yang Wang²
¹Department of Electronic Engineering, Shanghai Jiao Tong University
²Department of Computer Science, UC Santa Barbara
why2011btv@sjtu.edu.cn, {vvkulkarni,william}@cs.ucsb.edu

Abstract

We introduce a new method DOLORES for learning knowledge graph embeddings that effectively captures contextual cues and dependencies among entities and relations. First, we note that short paths on knowledge graphs comprising of chains of entities and relations can encode valuable information regarding their contextual usage. We operationalize this notion by representing knowledge graphs not as a collection of triples but as a collection of entity-relation chains, and learn embeddings for entities and relations using deep neural models that capture such contextual usage. In particular, our model is based on Bi-Directional LSTMs and learn deep representations of entities and relations from constructed entity-relation chains. We show that these representations can very easily be incorporated into existing models to significantly advance the state of the art on several knowledge graph prediction tasks like link prediction, triple classification, and missing relation type prediction (in some cases by at least 9.5%).

1 Introduction

Knowledge graphs (Dong et al., 2014) enable structured access to world knowledge and form a key component of several applications like search engines, question answering systems and conversational assistants. Knowledge graphs are typically interpreted as comprising of discrete triples of the form \((\text{entityA}, \text{relationX}, \text{entityB})\) thus representing a relation \(\text{relationX}\) between \text{entityA} and \text{entityB}. However, one limitation of only a discrete representation of triples is that it does not easily enable one to infer similarities and potential relations among entities which may be missing in the knowledge graph. Consequently, one popular alternative is to learn dense continuous representations of entities and relations by embedding them in latent continuous vector spaces, while seeking to model the inherent structure of the knowledge graph. Most knowledge graph embedding methods can be classified into two major classes: one class which operates purely on triples like RESCAL (Nickel et al., 2011), TRANSE (Bordes et al., 2013), DISTMULT (Yang et al., 2015), TRANSR (Ji et al., 2015), COMPLEX (Trouillon et al., 2016), CONVE (Dettmers et al., 2018) and the second class which seeks to incorporate additional information (like multi-hops) (Wang et al., 2017). Learning high-quality knowledge graph embeddings can be quite challenging given that (a) they need to effectively model the contextual usages of entities and relations (b) they would need to be useful for a variety of predictive tasks on knowledge graphs.

In this paper, we present a new type of knowledge graph embeddings called DOLORES that are both deep and contextualized. DOLORES learns both context-independent and context-dependent embeddings of entities and relations through a deep neural sequential model. Figure 1 illustrates the deep contextualized representations learned. Note that the contextually independent entity embeddings (see Figure 1a) reveal three clusters of entities: writers, philosophers, and musicians. The contextual dependent embeddings in turn effectively account for specific relations. In particular, the context-dependent representations under the relation nationality now nicely cluster the above entities by nationality namely Austrians, Germans, and British/Irish. Similarly Figure 1c shows contextual embeddings given the relation place-lived. Note that these embeddings correctly capture that even though Beethoven and Brahms being Germans, they lived in Vienna and are closer to other Austrian musi-
Figure 1: Context independent and dependent embeddings learned by DOLORES. (a) shows context-independent representations of writers (red), philosophers (green), and musicians (blue); (b) shows contextual embeddings with relation '/people/nationality': Austrians (green), Germans (blue), British/Irish (red). (c) shows contextual embeddings with relation '/people/place_lived/location', we can see that Beethoven and Brahms (in blue), though Germans (other Germans are in red), lived in Vienna, Austria (Austrians are in green) and lie in between Germans and Austrians.

Like most knowledge graph embeddings like TRANSD, TRANSE (Bordes et al., 2013; Ji et al., 2015) etc. which are typically learned using shallow models, the representations learned by DOLORES are deep: dependent on an entire path (rather than just a triple), are functions of internal states of a Bi-Directional LSTM and composed of representations learned at various layers potentially capturing varying degrees of abstractions. DOLORES is inspired by recent advances in learning word representations (word embeddings) from deep neural language models using Bi-Directional LSTMs (Peters et al., 2018). In particular, we derive connections between the work of Peters et al. (2018) who learn deep contextualized word embeddings from sentences using a Bi-Directional LSTM based language model and random walks on knowledge graphs. These connections enable us to propose new “deep contextualized” knowledge graph embeddings which we call DOLORES embeddings.

Knowledge Embeddings learned using DOLORES can easily be used as input representations for predictive models on knowledge graphs. More importantly, when existing predictive models use input representations for entities and relations, we can easily replace those representations with DOLORES representations and significantly improve the performance of existing models. Specifically, we show that DOLORES embeddings advance the state-of-the-art models on various tasks like link prediction, triple classification and missing relation type prediction.

To summarize, our contributions are as follows:

1. We present a new method DOLORES of learning deep contextualized knowledge graph embeddings using a deep neural sequential model.
2. These embeddings are functions of hidden states of the deep neural model and can capture both context-independent and context-dependent cues.
3. We show empirically that DOLORES embeddings can easily be incorporated into existing predictive models on knowledge graphs to advance the state of the art on several tasks like link prediction, triple classification, and missing relation type prediction.

2 Related Work

Extensive work exists on knowledge graph embeddings dating back to Nickel, Tresp, and Kriegel (2011) who first proposed RESCAL based on a matrix factorization approach. Bordes et al. (2013) advanced this line of work by proposing the first translational model TRANSE which seeks to relate the head and tail entity embeddings by modeling the relation as a translational vector. This culminated in a long series of new knowledge graph embeddings all based on the translational principle with various refinements (Wang et al., 2014; Lin et al., 2015; Ji et al., 2015; Yang et al., 2015; Trouillon et al., 2016; Nickel and Kiela, 2017; Minervini et al., 2017; Xiao et al., 2017; Ma et al., 2017; Chen and Zaniolo, 2017; Chen et al., 2018). Some recently proposed models like MANIFOLDE (Xiao et al., 2016) attempt to learn knowledge graph embeddings as a manifold while embeddings like HOLE (Nickel et al., 2011) derive inspiration from associative memories. Furthermore, with the success of neural models, models based on convolutional neural networks have
been proposed like (Dettmers et al., 2018; Shi and Weninger, 2017) to learn knowledge graph embeddings. Other models in this class of models include CONVKB (Nguyen et al., 2018b) and KB-GAN (Cai and Wang, 2018). There has been some work on incorporating additional information like entity types, relation paths etc. to learn knowledge graph representations. Palumbo et al. (2018) use NODE2VEC to learn embeddings of entities and items in a knowledge graph. A notable class of methods called “path-ranking” based models directly model paths between entities as features. Examples include Path Ranking Algorithm (PRA) (Lao et al., 2012), PTransE (Lin et al., 2015) and models based on recurrent neural networks (Nellakantan et al., 2015; Das et al., 2017). Besides, Das et al. (2018) propose a reinforcement learning method that addresses practical task of answering questions where the relation is known, but only one entity. Hartford et al. (2018) model interactions across two or more sets of objects using a parameter-sharing scheme.

While most of the above models except for the recurrent-neural net abased models above are shallow our model DOLORES differs from all of these works and especially that of Palumbo et al. (2018) in that we learn deep contextualized knowledge graph representations of entities and relations using a deep neural sequential model. The work that is closest to our work is that of Das et al. (2017) who directly use an RNN-based architecture to model paths to predict missing links. We distinguish our work from this in the following key ways: (a) First, unlike Das et al. (2017), our focus is not on path reasoning but on learning rich knowledge graph embeddings useful for a variety of predictive tasks. Moreover while Das et al. (2017) need to use paths generated from PRA that typically correlate with relations, our method has no such restriction and only uses paths generated by generic random walks greatly enhancing the scalability of our method. In fact, we incorporate DOLORES embeddings to improve the performance of the model proposed by Das et al. (2017). (b) Second, and most importantly we learn knowledge graph embeddings at multiple layers each potentially capturing different levels of abstraction. (c) Finally, while we are inspired by the work of Peters et al. (2018) in learning deep word representations, we build on their ideas by drawing connections between knowledge graphs and language modeling (Peters et al., 2018). In particular, we propose methods to use random walks over knowledge graphs in conjunction with the machinery of deep neural language modeling to learn powerful deep contextualized knowledge graph embeddings that improve the state of the art on various knowledge graph tasks.

3 Method and Models

3.1 Problem Formulation

Given a knowledge graph $G = (E, R)$ where $E$ denotes the set of entities and $R$ denotes the set of relations among those entities, we seek to learn $d$-dimensional embeddings of the entities and relations. In contrast to previous knowledge graph embedding methods like (Bordes et al., 2013; Wang et al., 2014; Ji et al., 2015; Lin et al., 2015; Trouillon et al., 2016) which are based on shallow models and operates primarily on triples, our method DOLORES uses a deep neural model to learn “deep” and “contextualized” knowledge graph embeddings.

Having formulated the problem, we now describe DOLORES. DOLORES consists of two main components:

1. **Path Generator** This component is responsible for generating a large set of entity-relation chains that reflect the varying contextual usages of entities and relations in the knowledge graph.

2. **Learner** This component is a deep neural model that takes as input entity-relation chains and learns entity and relation embeddings which are weighted linear combination of internal states of the model thus capturing context dependence.

Both of the above components are motivated by recent advances in learning deep representations of words in language modeling. We motivate this below and also highlight key connections that enable us to build on these advances to learn DOLORES knowledge graph embeddings.

3.2 Preliminaries

**Language Modeling** Recall that the goal of a language model is to estimate the likelihood of a sequence of words: $w_1, w_2, \ldots, w_n$ where each word $w_i$ is from a finite vocabulary $V$. Specifically, the goal of a forward language model is to
model $\Pr(w_i|w_1, w_2, \cdots, w_{i-1})$. While, traditionally this has been modeled using count-based “n-gram based” models (Manning and Schütze, 1999; Jurafsky, 2000), recently deep neural models like LSTMs and RNN’s have been used to build such language models. As noted by Peters et al. (2018), a forward language model implemented using an LSTM of “L” layers works as follows: At each position $k$, each LSTM layer outputs a context-dependent representation denoted by $h_{k,j}$ corresponding to the $j^{th}$ layer of the LSTM. The top-most layer of the LSTM is then fed as input to a softmax layer of size $|V|$ to predict the next token. Similarly, a backward language model which models $\Pr(w_i|w_{i+1}, w_{i+2}, \cdots, w_{n})$ can be implemented using a “backward” LSTM producing similar representations. A Bi-Directional LSTM just combines both forward and backward directions and seeks to jointly maximize the log-likelihood of the forward and backward directional language model objectives.

We note that these context-dependent representations learned by the LSTM at each layer have been shown to be useful as “deep contextual” word representations in various predictive tasks in natural language processing (Peters et al., 2018). In line with this trend, we will also use deep neural sequential models more specifically Bi-Directional LSTMs to learn DOLORES embeddings. We do this by generalizing this approach to graphs by noting connections first noted by Perozzi, Al-Rfou, and Skiena (2014).

### Connection between Random Walks on Graphs and Sentences in Language

Since the input to a language model is a large corpus or set of sentences, one can generalize language modeling approaches to graphs by noting that the analog of a sentence in graphs is a “random walk”. More specifically, note that a truncated random walk of length $T$ starting from a node “v” is analogous to a sentence and effectively captures the context of “v” in the network. More precisely, the same machinery used to learn representations of words in language models can now be adapted to learn deep contextualized representations of knowledge graphs.

This can easily be adapted to knowledge graphs by constructing paths of entities and relations. In particular, a random walk on a knowledge graph starting at entity $e_1$ and ending at entity $e_k$ is a sequence of the form $e_1, r_1, e_2, r_2, \cdots, e_k$ representing the entities and the corresponding relations between $e_1$ and $e_k$ in the knowledge graph. Moving forward we denote such a path of entities and relations by $q = (e_1, r_1, e_2, r_2, \cdots, e_k)$. We generate a large set of such paths from the knowledge graph $G$ by performing several random walks on it which in turn yields a corpus of “sentences” $S$ needed for “language modeling”.

### 3.3 DOLORES: Path Generator

Having motivated the model and discussed preliminaries, we now describe the first component of DOLORES – the path generator.

Let $S$ denote the set of entity-relation chains obtained by doing random walks in the knowledge graph. We adopt a component of NODE2VEC (Grover and Leskovec, 2016) to construct $S$. In particular, we perform a 2nd order random walk with two parameters $p$ and $q$ that determine the degree of breadth-first sampling and depth-first sampling. Specifically as Grover and Leskovec (2016) described, $p$ controls the likelihood of immediately revisiting a node in the walk whereas $q$ controls whether the walk is biased towards nodes close to starting node or away from starting node. We emphasize that while NODE2VEC has additional steps to learn dense continuous representations of nodes, we adopt only its first component to generate a corpus of random walks representing paths in knowledge graphs.

### 3.4 DOLORES: Learner

Having generated a set of paths on knowledge graphs representing local contexts of entities and relations, we are now ready to utilize the machinery of language modeling using deep neural networks to learn DOLORES embeddings.

While traditional language models model a sentence as a sequence of words, we adopt the same machinery to model knowledge graph embeddings as follows: (a) A word is an (entity, relation) tuple, (b) we model a sentence as a path consisting of (entity, relation) tuples. Note that we have already established how to generate such paths from the knowledge graph using the path generator component.

Given such paths, we would like to model the probability of an entity-relation pair given the history and future context by a Bi-Directional Long Short-Term Memory network. In particular, the
forward direction LSTM models:

$$\Pr([e_1, r_1], [e_2, r_2], \cdots, [e_N, r_N]) = \prod_{t=1}^{N} \Pr([e_t, r_t] | [e_1, r_1], [e_2, r_2], \cdots, [e_{t-1}, r_{t-1}]).$$

Similarly, the backward direction LSTM models:

$$\Pr([e_1, r_1], [e_2, r_2], \cdots, [e_N, r_N]) = \prod_{t=1}^{N} \Pr([e_t, r_t] | [e_{t+1}, r_{t+1}], \cdots, [e_N, r_N]).$$

Figure 2 illustrates this succinctly. At each time-step $t$, we deal with an entity-relation pair $[e_t, r_t]$. We first map one-hot vectors of the $e_t$ and $r_t$ to an embedding layer, concatenate them to obtain context-independent representations which are then passed through $L$ layers of a Bi-Directional LSTM. Each layer of LSTM outputs the pair’s context-dependent representation $h_t^{\rightarrow}$, where $i=1, 2, \cdots, L$. Finally, the output of the top layer of LSTM, $h_{t,L}$, is used to predict the next pair $[e_{t+1}, r_{t+1}]$ and $[e_{t-1}, r_{t-1}]$ respectively using a softmax layer. Formally, we jointly maximize the log likelihood of the forward and backward directions:

$$\sum_{t=1}^{N} \log \Pr([e_t, r_t] | [e_1, r_1], \cdots, [e_{t-1}, r_{t-1}] ; \Theta_F) + \sum_{t=1}^{N} \log \Pr([e_t, r_t] | [e_{t+1}, r_{t+1}], \cdots, [e_N, r_N] ; \Theta_B),$$

where $\Theta_F=\theta_x, \theta_{LSTM}, \theta_s$ corresponds to the parameters of the embedding layer, forward-direction LSTM and the softmax layer respectively. Similarly $\Theta_B=\theta_x, \theta_{LSTM}, \theta_s$ corresponds to the similar set of parameters for the backward direction. Specifically, note that we share the parameters for the embedding and softmax layer across both directions. We maximize Equation 3 by training the Bi-directional LSTMs using back-propagation through time.

**Extracting DOLORES embeddings from the learner** After having estimated the parameters of the DOLORES learner, we now extract the context-independent and context-dependent representations for each entity and relation and combine them to obtain DOLORES embeddings. More specifically, DOLORES embeddings are task specific combination of the context-dependent and context-independent representations learned by our learner. Note that our learner (which is an $L$-layer Bi-Directional LSTM) computes a set of $2L+1$ representations for each entity-relation pair which we denote by:

$$R_t = [x_t, h_{t,i}, h_{t,i} \rightarrow \leftarrow | i = 1, 2, \cdots, L],$$
Table 1: Summary of results of incorporating DOLORES embeddings on state-of-the-art models for various tasks. Note that in each case, simply incorporated DOLORES results in a significant improvement over the state of the art in various tasks like link prediction, triple classification and missing relation type prediction sometimes by as much as 9.5%.

| TASK                        | PREVIOUS SOTA | DOLORES+ BASELINE | INCREASE (ABSOLUTE/RELATIVE) |
|-----------------------------|---------------|-------------------|------------------------------|
| Link Prediction (head)      | (Nguyen et al., 2018b) 35.5 | 37.5 | 2.0 / 3.1% |
| Link Prediction (tail)      | (Nguyen et al., 2018b) 44.3 | 48.7 | 4.4 / 7.9% |
| Triple Classification       | (Nguyen et al., 2018b) 88.20 | 88.40 | 0.20 / 1.7% |
| Missing Relation Type       | (Das et al., 2017) 71.74 | 74.42 | 2.68 / 9.5% |

Table 2: Performance of incorporating DOLORES on state-of-the-art model for link prediction. Note that we consistently and significantly improve the current state of the art in both subtasks: head entity and tail entity prediction (in some cases by at least 9%). For all metrics except MR (mean rank) higher is better.

| METHOD                      | FB15K237 |               |               |               |               |
|-----------------------------|----------|---------------|---------------|---------------|---------------|
|                             | HEAD     | TAIL          | AVG           |               |               |
|                             | MRR      | MR | HITS@10    | MRR | MR | HITS@10    | MRR | MR | HITS@10    | MRR | MR | HITS@10    |
| TRANSE                      | 0.154    | 651 | 0.294       | 0.332 | 391 | 0.524       | 0.243 | 521 | 0.409       |       |     |            |
| CONVE                       | 0.204    | 375 | 0.366       | 0.408 | 189 | 0.594       | 0.306 | 283 | 0.480       |       |     |            |
| CONVKB (SOTA)               | 0.355    | 348 | 0.459       | 0.443 | 178 | 0.572       | 0.399 | 263 | 0.515       |       |     |            |
| CONVKB (+ DOLORES)          | 0.375    | 316 | 0.476       | 0.487 | 158 | 0.596       | 0.431 | 237 | 0.536       |       |     |            |
| IMPROVEMENT (RELATIVE %)    | 3.10%    | 9.20% | 3.14%       | 7.90% | 11.23% | 5.61%       | 5.32% | 9.89% | 4.33%       |       |     |            |

where \(x_t\) is the context-independent embedding and \(h_{t,i}, \overrightarrow{h}_{t,i}, \overleftarrow{h}_{t,i}\) correspond to the context-dependent embeddings from layer \(i\).

Given a downstream model, DOLORES learns a weighted linear combination of the components of \(R_i\) to yield a single vector for use in the embedding layer of the downstream model. In particular

\[
\text{DOLORES}_t = [x_t, \sum_{i=1}^{L} \lambda_i h_{t,i}],
\]

where we denote \(h_{t,i} = [\overrightarrow{h}_{t,i}, \overleftarrow{h}_{t,i}]\) and \(\lambda_i\) denote task specific learnable weights of the linear combination.

Incorporating DOLORES embeddings into existing predictive models on Knowledge Graphs

While it is obvious that our embeddings can be used as features for new predictive models, it is also very easy to incorporate our learned DOLORES embeddings into existing predictive models on knowledge graphs. The only requirement is that the model accepts as input, an embedding layer (for entities and relations). If a model fulfills this requirement (which is a large number of neural models on knowledge graphs do), we can just use DOLORES embeddings as a drop-in replacement. We just initialize the corresponding embedding layer with DOLORES embeddings. In our evaluation below, we show how to improve several state-of-the-art models on various tasks simply by incorporating DOLORES as a drop-in replacement to the original embedding layer.

4 Experiments

We evaluate DOLORES on a set of 4 different prediction tasks on knowledge graphs. In each case, simply adding DOLORES to existing state-of-the-art models improves the state of the art performance significantly (in some cases by at least 9.5%) which we show in Table 1. While we primarily show that we can advance the state-of-the-art model by incorporating DOLORES embeddings as a “drop-in” replacement, for the sake of completeness, we also report raw numbers of other strong baseline methods (like TransD, TransE, KBGAN, ConvE, and ConvKB) to place the results in context. We emphasize that our method is very generic and can be used to improve the performance of a large class of knowledge graph prediction models. In the remainder of the section, we briefly provide high-level overviews of each task and summarize results for all tasks considered.

4.1 Experimental Settings for DOLORES

Here, we outline our model settings for learning DOLORES embeddings. We generate 20 chains for each node in the knowledge graph, with the length of each chain being 21 (10 relations and 11
entities appear alternately)\(^1\). Our model uses \(L = 4\) LSTM layers with 512 units and 32 dimension projections (projected values are clipped element-wise to within \([-3, 3]\)). We use residual connections between layers and the batch size is set to 1024 during the training process. We train DOLORES for 200 epochs on corresponding datasets with dropout (with the dropout probability is set 0.1). Finally, we use Adam as the optimizer with appropriately chosen learning rates based on a validation set.

### 4.2 Evaluation Tasks

We consider three tasks, link prediction, triple classification, and predicting missing relation types (Das et al., 2017):

- **Link Prediction** A common task for knowledge graph completion is link prediction, aiming to predict the missing entity when the other two parts of a triplet \((h, r, t)\) are given. In other words, we need to predict \(t\) given \((h, r)\) – tail-entity prediction or predict \(h\) given \((r, t)\) – head entity prediction. In-line with prior work (Dettmers et al., 2018), we report results on link prediction in terms of Mean Reciprocal Rank (MRR), Mean Rank (MR) and Hits@10 on the FB15K-237 dataset in the filtered setting on both sub-tasks: (a) head entity prediction and (b) tail entity prediction. Our results are shown in Table 2. Note that the present state-of-the-art model, ConvKB achieves an MRR of \((0.375, 0.487)\) on the head and tail link prediction tasks. Observe that simply incorporating DOLORES significantly improves the head and tail entity prediction performance by 3.10% and 7.90% respectively. Similar improvements are also observed on other metrics like Mean Rank (MR: lower is better) and Hits@10 (higher is better).

- **Triple Classification** The task of triple classification is to predict whether a triple \((h, r, t)\) is correct or not. Triple classification is a binary classification task widely explored by previous work (Bordes et al., 2013; Wang et al., 2014; Lin et al., 2015). Since evaluation of classification needs negative triples, we choose WN11 and FB13, two benchmark datasets and report the results of our evaluation in Table 3. We note that the present state of the art is the ConvKB model. When we add DOLORES to the ConvKB model with our embeddings, observe that we improve the average performance of the state-of-the-art model ConvKB slightly by 0.20 points (from 88.20 to 88.40). We believe the improvement achieved by adding DOLORES is smaller in terms of absolute size because the state-of-the-art model already has excellent performance on this task (88.20) suggesting a much slower improvement curve.

| Method          | WN11 | FB13 | Avg. |
|-----------------|------|------|------|
| TRANSE          | 86.5 | 87.5 | 87.00|
| TRANSR          | 85.9 | 82.5 | 84.20|
| TRANDS          | 86.4 | 89.1 | 87.75|
| TRANSG          | 87.4 | 87.3 | 87.35|
| ConvKB (SOTA)   | 87.6 | 88.8 | 88.20|
| ConvKB (+ Dolores) | 87.5 | 89.3 | 88.40|

Table 3: Experimental results of triple classification on WN11 and FB13 test sets. TransE is implemented by Nguyen et al. (2018a). Except for ConvKB(+ Dolores), other results are from Nguyen et al. (2018a). Bold results are the best ones and underlined results are second-best.

- **Missing Relation Types** The goal of the third task is to reason on the paths connecting an entity pair to predict missing relation types. We follow Das et al. (2017) and use the same dataset released by Neelakantan, Roth, and McCallum (2015) which is a subset of FreeBase enriched with information from ClueWeb. The dataset consists of a set of triples \((e_1, r, e_2)\) and the set of paths connecting the entity pair \((e_1, e_2)\) in the knowledge graph. These triples are collected from ClueWeb by considering sentences that contain the entity pair in FreeBase. Neelakantan et al. (2015) infer the relation type by examining the phrase between two entities. We use the same evaluation criterion as used by Das et al. (2017) and report our results in Table 4. Note that the current state-of-the-art model from Das et al. (2017) yields a score of 71.74. Adding DOLORES to the model improves the score to 74.42 yielding a 9.5% improvement.

Altogether, viewing the results on various tasks...
holistically, we conclude that simply incorporating DOLORES into existing state-of-the-art models improves their performance and advances the state of the art on each of these tasks and suggests that our embeddings can be effective in yielding performance gains on a variety of predictive tasks.

4.3 Error Analysis

In this section, we conduct an analysis of the predictions made when using DOLORES on the link prediction tasks to gain insights into our learned embeddings. To do so, we group the test triples by the first component of their relation (the most abstract concept or level) and compute the mean rank of the tail entity output over each group. We compare this metric against what a simple baseline like TRANSE obtains. This enables us to identify overall statistical patterns that distinguish DOLORES embeddings from baseline embeddings like TRANSE, which in turn boosts the performance of link prediction.

Figure 3 shows the relation categories for which DOLORES performed the best and the worst relative to baseline TRANSE embeddings in terms of mean rank (lower is better). In particular, Figure 3a shows the categories where DOLORES performs the best and reveals categories like “food, user, olympics, organization” that are specific and tend to perform sub-optimally when the head entity is very generic and broad belonging to categories “base, common”. Please refer to Error Analysis section for detailed explanation and discussion.

![Figure 3](image)

(a) Best Prediction Categories for DOLORES

(b) Worst Prediction Categories for DOLORES

Table 4: Results of missing relation type prediction. RNN-Path-entity (Das et al., 2017) is the state of the art which yields an improvement of 9.5% (71.74 vs 74.42) on mean average precision (MAP) when incorporated with DOLORES.

| Model | MAP |
|-------|-----|
| PRA (Lao et al., 2011) | 64.43 |
| PRA + Bigram (Neelakantan et.al 2015) | 64.93 |
| RNN-Path (Dash et.al 2017) | 68.43 |
| RNN-Path-entity (Dash et.al 2017) SOTA | 71.74 |
| RNN-Path-entity (+DOLORES) | 74.42 |

Note that when the head entity is a very specific entity like Louis Costello, our method is very accurate at predicting the correct tail entity (in this case Comedian). TRANSE, on the other hand, makes very poor predictions on such cases. We believe that our method is able to model such cases better because our embeddings, especially for such specific entities, have captured the rich context associated with them from entire paths.

In contrast, Figure 3b shows the relation categories that DOLORES performs the worst relative to TRANSE. We note that these correspond to very broad relation categories like “common, base, media_common” etc. We list a few triples below to illustrate this point:

- (A serious man, film-release-region, Hong Kong)
- (Cabaret, film-genre, Film Adaptation)
- (Lou Costello, people-profession, Comedian)
Note that such instances are indeed very difficult. For instance, given a very generic entity like Psychology it is very difficult to guess that Yanni would be the expected tail entity. Altogether, our method is able to better model triples where the head entity is more specific compared to head entities which are very broad and general.

5 Conclusion

In this paper, we introduce DOLORES, a new paradigm of learning knowledge graph embeddings where we learn not only contextual independent embeddings of entities and relations but also multiple context-dependent embeddings each capturing a different layer of abstraction. We demonstrate that by leveraging connections between three seemingly distinct fields namely: (a) large-scale network analysis, (b) natural language processing and (c) knowledge graphs we are able to learn rich knowledge graph embeddings that are deep and contextualized in contrast to prior models that are typically shallow. Moreover, our learned embeddings can be easily incorporated into existing knowledge graph prediction models to improve their performance. Specifically, we show that our embeddings are not only a “drop-in” replacement for existing models that use embedding layers but also significantly improve the state-of-the-art models on a variety of tasks, sometimes by almost 9.5%. Furthermore, our method is inherently online and scales to large data-sets.

Our work also naturally suggests new directions of investigation and research into knowledge graph embeddings. One avenue of research is to investigate the utility of each layer’s entity and relation embeddings in specific learning tasks. As was noted by research in computer vision, deep representations learned on one dataset are effective and very useful in transfer-learning tasks (Huang et al., 2017). A natural line of investigation thus revolves around precisely quantifying the effectiveness of these learned embeddings across models and data-sets. Lastly, it would be interesting to see if such knowledge graph embeddings can be used in conjunction with natural language processing models used for relation extraction and named entity recognition from raw textual data.

Finally, in a broader perspective, our work introduces two new paradigms of modeling knowledge graphs. First, rather than view a knowledge graph as a collection of triples, we view it as a set of paths between entities. These paths can be represented as a collection of truncated random walks over the knowledge graph and encode rich contextual information between entities and relations. Second, departing from the hitherto well-established paradigm of mapping entities and relations to vectors in $\mathbb{R}^d$ via a mapping function, we learn multiple representations for entities and relations determined by the number of layers in a deep neural network. This enables us to learn knowledge graph embeddings that capture different layers of abstraction – both context-independent and context-dependent allowing for the development of very powerful prediction models to yield superior performance on a variety of prediction tasks.

References

Antoine Bordes, Nicolas Usunier, Alberto Garcia-Duran, Jason Weston, and Oksana Yakhnenko. 2013. Translating embeddings for modeling multi-relational data. In NIPS.

Liwei Cai and William Yang Wang. 2018. Kbgan: Adversarial learning for knowledge graph embeddings. In NAACL.

Muhao Chen, Yingtao Tian, Xuelu Chen, Zijun Xue, and Carlo Zaniolo. 2018. On2vec: Embedding-based relation prediction for ontology population. In Proceedings of the 2018 SIAM International Conference on Data Mining, pages 315–323. SIAM.

Muhao Chen and Carlo Zaniolo. 2017. Learning multi-faceted knowledge graph embeddings for natural language processing. In IJCAI.

Rajarshi Das, Shehzaad Dhuliawala, Manzil Zaheer, Luke Vilnis, Ishan Durugkar, Akshay Krishnamurthy, Alex Smola, and Andrew McCallum. 2018. Go for a walk and arrive at the answer: Reasoning over paths in knowledge bases using reinforcement learning. In ICLR.

Rajarshi Das, Arvind Neelakantan, David Belanger, and Andrew McCallum. 2017. Chains of reasoning over entities, relations, and text using recurrent neural networks. In EACL.

Tim Dettmers, Pasquale Minervini, Pontus Stenetorp, and Sebastian Riedel. 2018. Convolutional 2d knowledge graph embeddings. In AAAI.
Xin Dong, Evgeniy Gabrilovich, Geremy Heitz, Wilko Horn, Ni Lao, Kevin Murphy, Thomas Strohmann, Shaohua Sun, and Wei Zhang. 2014. Knowledge vault: A web-scale approach to probabilistic knowledge fusion. In KDD.

Aditya Grover and Jure Leskovec. 2016. node2vec: Scalable feature learning for networks. In KDD.

Jason Hartford, Devon Graham, Kevin Leyton-Brown, and Siamak Ravanbakhsh. 2018. Deep models of interactions across sets. arXiv preprint arXiv:1803.02879.

Zhongling Huang, Zongxu Pan, and Bin Lei. 2017. Transfer learning with deep convolutional neural network for sar target classification with limited labeled data. Remote Sensing.

Guoliang Ji, Shizhu He, Liheng Xu, Kang Liu, and Jun Zhao. 2015. Knowledge graph embedding via dynamic mapping matrix. In ACL-IJCNLP.

Dan Jurafsky. 2000. Speech & language processing. Pearson Education India.

Ni Lao, Tom Mitchell, and William W Cohen. 2011. Random walk inference and learning in a large scale knowledge base. In EMNLP.

Yankai Lin, Zhiyuan Liu, Maosong Sun, Yang Liu, and Xuan Zhu. 2015. Learning entity and relation embeddings for knowledge graph completion. In EMNLP.

Shiheng Ma, Jianhui Ding, Weijia Jia, Kun Wang, and Minyi Guo. 2017. Transt: Type-based multiple embedding representations for knowledge graph completion. In Joint European Conference on Machine Learning and Knowledge Discovery in Databases, pages 717–733. Springer.

Christopher D Manning and Hinrich Schütze. 1999. Foundations of statistical natural language processing. MIT press.

Pasquale Minervini, Luca Costabello, Emir Muñoz, Vít Nováček, and Pierre-Yves Vandenbussche. 2017. Regularizing knowledge graph embeddings via equivalence and inversion axioms. In Joint European Conference on Machine Learning and Knowledge Discovery in Databases, pages 668–683. Springer.

Arvind Neelakantan, Benjamin Roth, and Andrew McCallum. 2015. Compositional vector space models for knowledge base completion. In ACL-IJCNLP.

Dai Quoc Nguyen, Dat Quoc Nguyen, Tu Dinh Nguyen, and Dinh Phung. 2018a. A convolutional neural network-based model for knowledge base completion and its application to search personalization. Semantic Web, (Preprint).

Dai Quoc Nguyen, Tu Dinh Nguyen, Dat Quoc Nguyen, and Dinh Phung. 2018b. A novel embedding model for knowledge base completion based on convolutional neural network. In NAACL.

Maximilian Nickel and Douwe Kiela. 2017. Poincaré embeddings for learning hierarchical representations. In NIPS.

Maximilian Nickel, Volker Tresp, and Hans-Peter Kriegel. 2011. A three-way model for collective learning on multi-relational data. In ICML.

Enrico Palumbo, Giuseppe Rizzo, Raphaël Troncy, Elena Baralis, Michele Osella, and Enrico Ferro. 2018. Knowledge graph embeddings with node2vec for item recommendation. In European Semantic Web Conference. Springer.

Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. 2014. Deepwalk: Online learning of social representations. In KDD.

Matthew Peters, Mark Neumann, Mohit Iyyer, Matt Gardner, Christopher Clark, Kenton Lee, and Luke Zettlemoyer. 2018. Deep contextualized word representations. In NAACL.

Baoxu Shi and Tim Weninger. 2017. Proje: Embedding projection for knowledge graph completion. In AAAI, volume 17, pages 1236–1242.

Théo Trouillon, Johannes Welbl, Sebastian Riedel, Éric Gaussier, and Guillaume Bouchard. 2016. Complex embeddings for simple link prediction. In ICML.

Quan Wang, Zhendong Mao, Bin Wang, and Li Guo. 2017. Knowledge graph embedding: A survey of approaches and applications. IEEE Transactions on Knowledge and Data Engineering.

Zhen Wang, Jianwen Zhang, Jianlin Feng, and Zheng Chen. 2014. Knowledge graph embedding by translating on hyperplanes. In AAAI.

Han Xiao, Minlie Huang, and Xiaoyan Zhu. 2017. Ssp: Semantic space projection for knowledge graph embedding with text descriptions. In AAAI, volume 17, pages 3104–3110.

Han Xiao, Minlie Huang, and Xiaoyan Zhu. 2016. From one point to a manifold: Knowledge graph embedding for precise link prediction. In IJCAI.

Bishan Yang, Wen-tau Yih, Xiaodong He, Jianfeng Gao, and Li Deng. 2015. Embedding entities and relations for learning and inference in knowledge bases. In ICLR.