Modeling Relational Data with Graph Convolutional Networks

Michael Schlichtkrull*

University of Amsterdam m.s.schlichtkrull@uva.nl

Thomas N. Kipf*

University of Amsterdam t.n.kipf@uva.nl

Peter Bloem

VU Amsterdam p.bloem@vu.nl

Rianne van den Berg

University of Amsterdam r.vandenberg@uva.nl

Ivan Titov

University of Amsterdam titov@uva.nl

Max Welling

University of Amsterdam, CIFAR[†] m.welling@uva.nl

Abstract

Knowledge bases play a crucial role in many applications, for example question answering and information retrieval. Despite the great effort invested in creating and maintaining them, even the largest representatives (e.g., Yago, DBPedia or Wikidata) are highly incomplete. We introduce relational graph convolutional networks (R-GCNs) and apply them to two standard knowledge base completion tasks: link prediction (recovery of missing facts, i.e. subject-predicate-object triples) and entity classification (recovery of missing attributes of entities). R-GCNs are a generalization of graph convolutional networks, a recent class of neural networks operating on graphs, and are developed specifically to deal with highly multi-relational data, characteristic of realistic knowledge bases. Our methods achieve competitive results on standard benchmarks for both tasks.

1 Introduction

Knowledge bases organize and store factual knowledge and enable a wide variety of applications, including question answering [41, 1, 33, 16, 2, 10] and information retrieval [21, 7, 39, 38]. Even the largest of knowledge bases (e.g., DBPedia, Wikidata or Yago), despite enormous effort invested in their maintenance, are incomplete, and the lack of coverage harms downstream applications. Predicting missing information in knowledge bases is the main focus of statistical relational learning (SRL).

In this work, as in much previous work on SRL, we assume that knowledge bases store collections of triples of the form (subject, predicate, object). Consider, for example, the triple (*Mikhail Baryshnikov*, *educated_at*, *Vaganova Academy*), where we will refer to *Baryshnikov* and *Vaganova Academy* as entities and to *educated_at* as a relation. Additionally, we assume that entities are labeled with types (e.g., *Vaganova Academy* is marked as a *university*). It is convenient to represent knowledge bases as directed labeled multigraphs with entities corresponding to nodes and triples encoded by labeled edges (see Figure 1).

In this work, we consider two fundamental SRL tasks: link prediction (recovery of missing triples) and entity classification (assigning types to entities). In order to recover missing information, a statistical model needs to exploit regularities in the graphs. In our example, it should capture that having received the Vilcek prize (an award honoring contributions of immigrants to the US society) implies having the US citizenship, or graduating from the Vaganova Academy probably means that

^{*}Equal contribution.

[†]Canadian Institute for Advanced Research

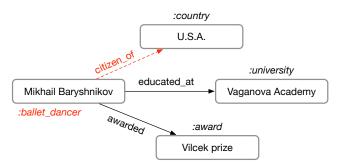


Figure 1: A knowledge base fragment: The nodes are entities, the edges are relations labeled with their types, the nodes are labeled with entity types (e.g., *university*). The edge and the node shown in red are the missing information to be inferred.

the entity is a ballet dancer. In other words, the model either decides on the label of a node or predicts a link between two nodes, relying on the neighborhood of these nodes in the graph. In order to induce informative latent feature representations of the nodes encoding relevant properties of their neighborhoods, we use graph convolutional networks (GCNs), a recent class of neural networks operating on graphs [4, 11, 9, 19]. GCNs have been shown very effective for semi-supervised node classification in undirected unlabeled graphs and consistently show competitive performance even for very large graphs, unlike, for example, walk-based models [19]. In this work, we introduce relational GCNs (R-GCNs). R-GCNs are specifically designed to deal with highly multi-relational data, characteristic of realistic knowledge bases.

Our entity classification model, similarly to Kipf and Welling [19], uses softmax classifiers at each node in the graph. The classifiers take node representations supplied by an R-GCN and predict the labels. The model, including R-GCN parameters, is learned by optimizing the cross-entropy loss.

Our link prediction model can be regarded as an autoencoder consisting of (1) an encoder: an R-GCN producing latent feature representations of entities, and (2) a decoder: a tensor factorization model exploiting these representations to predict labeled edges. Though in principle the decoder can rely on any type of factorization (or generally any scoring function), we use one of the simplest and most effective factorization methods: DistMult [40]. We observe that our method achieves competitive results on standard benchmarks, outperforming, among other baselines, direct optimization of the factorization (i.e. vanilla DistMult). Interestingly, behaviors of DistMult and the DistMult-based GCN model are quite different. Though DistMult has an edge over the GCN autoencoder for entities with few neighbors, the autoencoder substantially outperforms DistMult in other situations. Given their complementary properties, it is natural to combine them and, as we see in our experiments, this results in substantial performance gains.

The main contributions are as follows. To the best of our knowledge, we are the first to show that the GCN framework can be applied to modeling relational data, specifically to link prediction and entity classification tasks. Secondly, we introduce a parameter sharing technique and use it within R-GCNs, enabling us to apply R-GCNs to multigraphs with a large number of relations.

2 Relational Graph Convolutional Networks

In this work, we consider a non-linear, multi-layer convolutional model that operates directly on directed and labeled multi-graphs $G = (\mathcal{V}, \mathcal{E}, \mathcal{R})$ with nodes (entities) $v_i \in \mathcal{V}$ and labeled edges (relations) $(v_i, r, v_j) \in \mathcal{E}$, where $r \in \mathcal{R}$ is a relation type³.

We refer to this model as a Relational Graph Convolutional Network (R-GCN), as it can be seen as a practical generalization of (first-order) Graph Convolutional Networks (GCNs) [11, 19] to directed relational graphs.

³We consider a directed relation such as *born_in* and its counterpart of inverse direction as separate elements in the set of relations \mathcal{R}_{λ} i.e. \mathcal{R}_{λ} includes a relation both in canonical and in inverse direction.

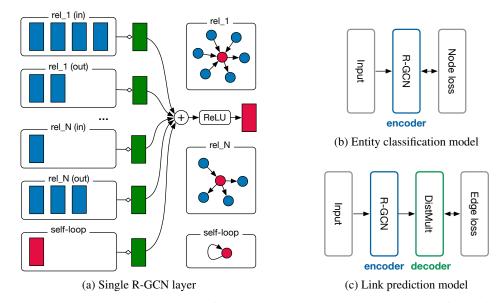


Figure 2: (a) R-GCN per-layer update for a single graph node (in red). Activations from neighboring nodes (blue) are gathered and then transformed according to (2) for each relation type individually (for both in- and outgoing edges). The resulting representation (green) is accumulated in a (normalized) sum and passed through an activation function (such as the ReLU). This per-node update can be computed in parallel with shared parameters across the whole graph. (b) Depiction of an R-GCN model for entity classification with a per-node loss function. (c) Link prediction model with an R-GCN encoder (interspersed with fully-connected/dense layers) and a DistMult decoder that takes pairs of hidden node representations and produces a score for every (potential) edge in the graph. The loss is evaluated per edge.

In each R-GCN layer, hidden state information is propagated across edges of the graph, while taking into account the type (relation) and direction of an edge. A single layer of this neural network model takes the following form:

$$h_i^{(l+1)} = \sigma \left(\sum_{r \in \mathcal{R}} \sum_{j \in \mathcal{N}_i^r} \frac{1}{c_{i,r}} W_r^{(l)} h_j^{(l)} + W_0^{(l)} h_i^{(l)} \right), \tag{1}$$

where $h_i^{(l)} \in \mathbb{R}^{d^{(l)}}$ is the hidden state of node v_i in the l-th layer of the neural network, with $d^{(l)}$ being the dimensionality of this layer's representations. $\sigma(\cdot)$ denotes a non-linear activation function such as the linear rectifier $\mathrm{ReLU}(\cdot) = \mathrm{max}(0,\cdot)$ and $c_{i,r}$ is a problem-specific normalization constant. \mathcal{N}_i^r denotes the set of neighbor indices of node i under relation $r \in \mathcal{R}$. $W_r^{(l)}$ (and $W_0^{(l)}$ in the same way) are defined as follows:

$$W_r^{(l)} = \sum_{b=1}^B a_{rb}^{(l)} V_b^{(l)}, \tag{2}$$

i.e. as a linear combination of basis transformations $V_b^{(l)} \in \mathbb{R}^{d^{(l+1)} \times d^{(l)}}$ with coefficients $a_{rb}^{(l)}$. By introducing a suitable normalization constant $c_{i,r}$ (such as $c_{i,r} = |\mathcal{N}_i^r|$), node activations can be kept on a similar scale across the graph, which can be crucial for modeling scale-free networks or graphs with very wide node degree distributions. The R-GCN model is depicted in Figure 2a.

The layer-wise propagation rule of the R-GCN model can be understood as a form of information propagation (and transformation) across edges of the graph. Each relation corresponds to a different transformation, given by a linear combination of a pre-defined number of basis transformations (2). Both the coefficients $a_{rb}^{(l)}$ and the basis transformations $V_b^{(l)}$ are trainable model parameters and are shared over all locations in the graph in the same way as filter parameters are shared in a convolutional neural network for, e.g., image data.

The basis function decomposition (2) can be seen as a form of effective weight sharing between different relation types. This reduces the number of parameters needed to learn for highly multi-relational data (such as realistic knowledge bases). At the same time, we expect that this parameterization can alleviate overfitting on rare relations, as parameter updates are shared between both rare and more frequent relations.

The overall R-GCN model then takes the following form: We stack L layers as defined in (1) – the output of the previous layer being the input to the next layer. The input to the first layer can be chosen as a unique one-hot vector for each node in the graph if no other features are present. While we only consider such a featureless approach in this work, we note that it was shown in [19] that it is possible for this class of models to make use of pre-defined feature vectors (e.g. a bag-of-words description of a document associated with a specific node).

3 Link prediction

Link prediction deals with prediction of new facts (i.e. triples (subject, relation, object)). Formally, the knowledge base is represented by a directed, labeled graph $G = (\mathcal{V}, \mathcal{E}, \mathcal{R})$. Rather than the full set of edges \mathcal{E} , we are given only an incomplete subset $\hat{\mathcal{E}}$. The task is to assign scores f(s, r, o) to possible edges (s, r, o) in order to determine how likely those edges are to belong to \mathcal{E} .

In order to tackle this problem, we introduce a graph auto-encoder model, comprised of an entity encoder and a scoring function (decoder). The encoder maps each entity $v_i \in \mathcal{V}$ to a real-valued vector $e_i \in \mathbb{R}^d$. The decoder reconstructs edges of the graph relying on the vertex representations; in other words, it scores (subject, relation, object)-triples through a function $s: \mathbb{R}^d \times \mathcal{R} \times \mathbb{R}^d \to \mathbb{R}$. Most existing approaches to link prediction (for example, tensor and neural factorization methods [34, 23, 36, 40, 37]) can be interpreted under this framework. The crucial distinguishing characteristic of our work is the reliance on an encoder. Whereas most previous approaches use a single, real-valued vector e_i for every $v_i \in \mathcal{V}$ optimized directly in training, we compute representations through an R-GCN encoder with $e_i = h_i^{(L)}$, similar to the graph auto-encoder model introduced in [18] for unlabeled undirected graphs. Our full link prediction model is schematically depicted in Figure 2c.

In our experiments, we use the DistMult factorization [40] as the scoring function, which is known to perform well on standard link prediction benchmarks when used on its own. In DistMult, every relation r is associated with a diagonal matrix $R_r \in \mathbb{R}^{d \times d}$ and a triple (s,r,o) is scored as:

$$f(s,r,o) = e_s^T R_r e_o. (3)$$

As in previous work on factorization [40, 37], we estimate the model through negative sampling. For each observed example we sample ω negative ones. We sample by randomly corrupting either the subject or the object of each positive example. We use the cross-entropy loss to push the model to score observable triples higher than the negative ones:

$$\mathcal{L} = -\frac{1}{(1+\omega)|\hat{\mathcal{E}}|} \sum_{(s,r,o,y)\in\mathcal{T}} y \log \sigma \big(f(s,r,o)\big) + (1-y) \log \big(1 - \sigma \big(f(s,r,o)\big)\big), \tag{4}$$

where \mathcal{T} is the total set of real and corrupted triplets, σ is the logistic sigmoid function, and y is an indicator set to y=1 for positive triples and y=0 for negative ones.

4 Entity classification

For (semi-)supervised classification of nodes (entities), we simply stack R-GCN layers of the form (1), while using a $\operatorname{softmax}(\cdot)$ activation (per node) on the output of the last layer. As proposed in [19], we evaluate the following cross-entropy loss on all labeled nodes (while ignoring unlabeled nodes):

$$\mathcal{L} = -\sum_{i \in \mathcal{Y}} \sum_{k=1}^{K} t_{ik} \ln h_{ik}^{(L)},$$
 (5)

where \mathcal{Y} is the set of node indices that have labels and $h_{ik}^{(L)}$ is the k-th entry of the network output for the i-th labeled node. t_{ik} denotes its respective ground truth label. In practice, we train the model using (full-batch) gradient descent techniques. A schematic depiction of our entity classification model is given in Figure 2b.

5 Empirical evaluation

5.1 Link prediction experiments

Dataset	#Entities	#Relations	#Train edges	#Validation edges	#Test edges
WN18	40,943	18	141,442	5,000	5,000
FB15K	14,951	1,345	483,142	50,000	59,071

Table 1: Number of entities and relations (i.e. relation types) along with the number of edges per split for the two datasets.

We evaluate our model on the WordNet (WN18) dataset, and on the Freebase (FB15K) dataset. WN18 is a subset of WordNet, containing lexical relations between words. FB15k is a subset of Freebase, a curated database of relations between entities. In both cases, we use the train, test, and validation splits first introduced by Bordes et al. [3]. Characteristics of the two datasets are summarized in Table 1.

All parameter selection was done on the validation set of FB15k. The normalization constant is defined as $c_{i,r} = c_i = \sum_r |\mathcal{N}_i^r|$, in other words, the normalization is applied across relation types. We use the Adam optimizer [17] with a learning rate of 0.01. The dimensionality of hidden states is set to 200. We use l2 regularization on the decoder with a penalty of 0.01. We use an edge dropout rate of 0.2 for self-loop, and of 0.4 for other edges. Dropout is applied before normalization. We use one layer of convolution, as we found it to yield the best performance. For our baseline, we found that parameters from Trouillon et al. [37] work best, though to make the systems comparable we keep the same dimensionality and the number of negative samples (i.e. $\omega=1$). We use full-batch optimization for both the baseline and our model.

We ran the link prediction experiments using a Titan X GPU. The baseline (DistMult) and R-GCN both reached the stopping criterion (validation MRR) after approximately 5,000 epochs, corresponding to approximately two hours for DistMult and three hours for R-GCN (for the larger FB15K dataset).

As standard in the literature, we provide results using two evaluation metrics: $mean\ reciprocal\ rank\ (MRR)$ and $Hits\ at\ n\ (H@n)$. As described in Bordes et al. [3], both metrics can be computed in a raw and a filtered setting. We report both filtered and raw MRR (with filtered MRR typically considered more reliable), and filtered Hits at 1, 3, and 10.

Model	MRR
DistMult	0.612
R-GCN (1)	0.641
R-GCN (2)	0.657
R-GCN (5)	0.639

Figure 3: Comparison of different GCN-variants on Freebase validation data. R-GCN (*B*) refers to R-GCN with *B* basis functions. We include the baseline performance for reference.

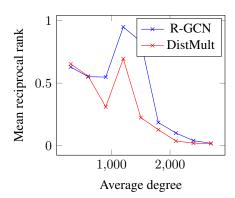


Figure 4: Mean reciprocal rank on the Freebase validation data as a function of the node degree (average of subject and object).

The natural baseline for our experiments is direct optimization of *DistMult* [40]. As described in Section 3, DistMult – in addition to performing well on standard benchmarks – corresponds to a version of our model with fixed entity embeddings instead of using the R-GCN encoder. In Table 3, we compare the performance of encoder configurations with different number of basis functions. We found R-GCN with two basis matrices yields the best results and outperforms the baseline.

To better understand the behavior of the R-GCN encoder, we plot the performance of the best R-GCN model and the baseline (DistMult) as functions of degree of nodes corresponding to entities in the

	FB15k				WN18					
MRR		Hits @		MRR		Hits @				
Model	Raw	Filtered	1	3	10	Raw	Filtered	1	3	10
DistMult	0.248	0.634	0.522	0.718	0.814	0.526	0.813	0.701	0.921	0.943
R-GCN	0.251	0.651	0.541	0.736	0.825	0.553	0.814	0.686	0.928	0.955
R-GCN+	0.262	0.696	0.601	0.760	0.842	0.561	0.819	0.697	0.929	0.964
CP*	0.152	0.326	0.219	0.376	0.532	0.075	0.058	0.049	0.080	0.125
TransE*	0.221	0.380	0.231	0.472	0.641	0.335	0.454	0.089	0.823	0.934
HolE**	0.232	0.524	0.402	0.613	0.739	0.616	0.938	0.930	0.945	0.949
ComplEx*	0.242	0.692	0.599	0.759	0.840	0.587	0.941	0.936	0.945	0.947

Table 2: Results on the Freebase and WordNet datasets. Results marked (*) taken from [37]. Results marks (**) taken from [26].

considered triple (namely, the average of degrees for the subject and object entities). As the R-GCN encoder is designed to capture context, we expect our model to perform better for nodes with high degree, where contextual information is abundant. In Figure 4, we see exactly that effect: while DistMult outperforms R-GCN by a slight margin on low-degree nodes, R-GCN performs much better on high-degree ones.

Observing that the strengths of the two models are complementary, we combine them. We define $f(s,r,t)_{\text{R-GCN+}} = \alpha f(s,r,t)_{\text{R-GCN}} + (1-\alpha)f(s,r,t)_{\text{DistMult}}$. The mixing ratio α was set to 0.4, chosen on the FB15k development dataset.

We now proceed to evaluate the R-GCN model and the combination model (R-GCN+) on test sets of the two datasets. The results can be seen in Table 2. As far as we are aware, ComplEx [37] and HolE [26] are the best performing methods on FB15k and WN18, respectively. ComplEx is a generalization of DistMult to the complex domain (more appropriate for modeling asymmetric relations), while HolE replaces the vector-matrix product with circular correlation. We include comparisons with these factorizations and with two classic approaches to the problem (CP [15] and TransE [3]). The choice of the factorization method is essentially orthogonal to a decision to use a R-GCN encoder or not: in principle, any factorization can be incorporated as a decoder in our R-GCN autoencoder. We leave this for future work.

On the Freebase dataset, R-GCN and R-GCN+ both outperform the baseline; R-GCN+ by a much larger margin. Interestingly, R-GCN+ yields better performance than ComplEx, even though the R-GCN decoder (DistMult) does not explicitly model asymmetry in relations, as opposed to ComplEx. It suggests that combining the R-GCN encoder and ComplEx may be promising. On Wordnet, R-GCN shows performance similar to the baseline, while R-GCN+ performs slightly better.

5.2 Entity classification experiments

For entity classification, we evaluate our model on three knowledge graph datasets [30]: AIFB, MUTAG and BGS. In each dataset the targets to be classified are properties of a group of entities represented as nodes. The exact statistics of the datasets can be found in Table 3. For a more detailed description of the datasets the reader is referred to Ristoski et al. [30].

As a baseline for our experiments, we compare against recent state-of-the-art classification results from RDF2Vec embeddings [31], Weisfeiler-Lehman kernels (WL) [8], and hand-designed feature extractors (Feat) [28]. RDF2Vec samples random walks on labeled graphs which are then processed using the Skipgram [24] model to generate entity embeddings, used for subsequent classification. See [31] for an in-depth description and discussion of these baseline approaches. Baseline results are reported as accuracy averaged over 10-fold stratified cross-validation.

We report performance of a 2-layer R-GCN entity classification model in terms of mean 10-fold stratified cross-validation accuracy, averaged over 10 repeated runs with random weight initializations.

Dataset	#Entities	#Relations	#Edges	#Labeled entities	#Classes
AIFB	8,285	45	29,043	176	4
MUTAG	23,644	23	74,227	340	2
BGS	333,845	103	916,199	146	2

Table 3: Number of entities, relations, edges and classes along with the number of labeled entities for each of the datasets. Labeled entities denotes the subset of entities that have labels and that are to be classified. Unless otherwise noted, we divide the labeled part of the dataset according to 10-fold stratified cross-validation or according to the official train/test benchmark splits from [30]. For the latter, we further use 5% of the training set for validation and train on both the training and the validation splits (i.e. the on the original training benchmark split) to obtain the final result on the respective test splits.

Results⁴ are summarized in Table 4. Via hyperparameter optimization on the validation splits, we found the original set of hyperparameters proposed in [19] for semi-supervised node classification with GCNs to generalize well to this setting, with the exception of BGS, where we found a higher dropout rate of 0.9 to work best. Otherwise, hyperparameters are chosen as follows: 30 (number of epochs), 10 (number of basis functions), 0.5 (dropout rate after first layer), $5 \cdot 10^{-4}$ (l2 penalty on first layer), 16 (number of hidden units), and $c_{i,r} = |\mathcal{N}_i^r|$ (normalization constant). We use the Adam optimizer [17] with a learning rate of 0.01.

All entity classification experiments were run on a single CPU workstation with a 16-core Intel Xeon CPU E5-2640 v3 @ 2.60GHz and 64GB of memory. Our entity classification model is implemented in keras [6] in conjunction with Theano [35] as backend. We make use of efficient sparse matrix operations wherever applicable.

Model	AIFB	MUTAG	BGS
Feat [28]	88.57	73.53	86.50
WL [8]	89.25	94.29	91.05
RDF2Vec [31]	93.41	96.18	96.33
R-GCN	95.74	66.40	84.70
R-GCN*	94.16	68.97	79.65

Table 4: Entity classification results in percent accuracy (10-fold stratified cross-validation). All baseline results are taken from [31], where we always choose their best-performing model variant. (*) denotes results on the benchmark test split from [30].

Our model achieves competitive performance on the AIFB dataset, but lacks behind the baseline models on both MUTAG and BGS by a substantial margin. We suspect that the inability of our model to fit the latter two datasets could potentially arise from our choice of normalization. This choice renders the model insensitive to the number of neighbors, which might be an essential feature for the MUTAG and BGS datasets. We will investigate this issue and other choices of normalization in future work.

6 Related Work

6.1 Relational modeling

Our encoder-decoder approach to link prediction relies on DistMult [40] in the decoder, a special and simpler case of the RESCAL factorization [27], more effective than the original RESCAL in the context of multi-relational knowledge bases. Numerous alternative factorizations have been

⁴In an earlier version of this paper, we performed experiments for entity classification on the raw versions of the AIFB, MUTAG and BGS datasets hosted at http://dws.informatik.uni-mannheim.de/en/research/a-collection-of-benchmark-datasets-for-ml without preprocessing. The raw datasets contain relations which were used to generate labels for the benchmark train/test splits from [30]. In this version of the paper, we remove these relations from the datasets, as otherwise our model is able to pick up this signal and classify at close to 100% accuracy. It is our understanding that the authors of [31] followed the same procedure.

proposed and studied in the context of SRL, including both (bi-)linear and nonlinear ones (e.g., [3, 34, 5, 26, 37]). Many of these approaches can be regarded as modifications or special cases of classic tensor decomposition methods such as CP or Tucker; for a comprehensive overview of tensor decomposition literature we refer the reader to Kolda and Bader [20].

Incorporation of paths between entities in knowledge bases has recently received considerable attention. We can roughly classify previous work into (1) methods creating auxiliary triples, which are then added to the learning objective of a factorization model [14, 12]; (2) approaches using paths (or walks) as features when predicting edges [23]; or (3) doing both at the same time [25, 36]. The first direction is largely orthogonal to ours, as we would also expect improvements from adding similar terms to our loss (in other words, extending our decoder). The second research line is more comparable; R-GCNs provide a computationally cheaper alternative to these path-based models. Direct comparison is somewhat complicated as path-based methods used different datasets (e.g., sub-sampled sets of walks from a knowledge base).

6.2 Neural networks on graphs

Our R-GCN model can be seen as an extension of existing work in the field of neural networks on graphs. (Recurrent) graph neural networks were first introduced in [13, 32] and later extended with modern practices for training recurrent neural networks in [22]. These models naturally support labeled graphs, they are however limited to fixed-size node representations due to their recurrent nature.

Graph convolutional networks [4, 11, 9, 19] are a related line of research that allow for layer-wise changes in representation size. These models were so far only considered for undirected and unlabeled graphs. Our encoder model extends graph convolutional networks by incorporating support for multiple relation types, directed edges and a form of efficient weight sharing for graphs with a large number of relation types.

Column Networks [29] take a related approach by introducing a hybrid recurrent/convolutional model for relational graphs that makes use of highway connections, yet lacks weight sharing for relations and therefore does not scale favorably to real-world datasets such as the ones considered here.

7 Conclusions

We have introduced relational graph convolutional networks (R-GCNs) and demonstrated their effectiveness in the context of two standard statistical relation modeling problems: link prediction and entity classification. For the link prediction problem, the R-GCN model with DistMult factorization as the decoding component outperformed direct optimization of the factorization model, and achieved competitive results on standard link prediction benchmarks. For the entity classification problem, our model outperforms previous methods on the AIFB dataset by a significant margin, yet lacks behind even a simple feature-based approach on two other datasets (MUTAG and BGS). It remains to be seen whether this is due to the specific choice of normalization in our model, which makes R-GCNs invariant to the node degree—thereby making the model insensitive to a potentially essential feature for some datasets.

There are several ways in which our work could be extended. For example, the graph autoencoder model could be considered in combination with other factorization models, such as ComplEx [37], which can be better suited for modeling asymmetric relations. It is also straightforward to integrate entity features in R-GCNs, which would be beneficial both for link prediction and entity classification problems. Lastly, to gain a better understanding of how basis transformations are used to represent knowledge base relations, it would be interesting to perform a more thorough analysis of learned relation embeddings.

Acknowledgments

We would like to thank Diego Marcheggiani, Ethan Fetaya, and Christos Louizos for helpful discussions and comments. This project is supported by the European Research Council (ERC StG BroadSem 678254), the SAP Innovation Center Network and the Dutch National Science Foundation (NWO VIDI 639.022.518).

References

- [1] Junwei Bao, Nan Duan, Ming Zhou, and Tiejun Zhao. Knowledge-based question answering as machine translation. In *Proceedings of the 52nd Annual Meeting of the Association for Computational Linguistics*, pages 967–976. Association for Computational Linguistics, 2014.
- [2] Antoine Bordes, Nicolas Usunier, Sumit Chopra, and Jason Weston. Large-scale simple question answering with memory networks. *arXiv* preprint arXiv:1506.02075, 2015.
- [3] Antoine Bordes, Nicolas Usunier, Alberto Garcia-Duran, Jason Weston, and Oksana Yakhnenko. Translating embeddings for modeling multi-relational data. In *Advances in neural information processing systems*, pages 2787–2795, 2013.
- [4] Joan Bruna, Wojciech Zaremba, Arthur Szlam, and Yann LeCun. Spectral networks and locally connected networks on graphs. In *International Conference on Learning Representations (ICLR)*, 2014.
- [5] Kai-Wei Chang, Wen tau Yih, Bishan Yang, and Chris Meek. Typed Tensor Decomposition of Knowledge Bases for Relation Extraction. In EMNLP, 2014.
- [6] François Chollet. keras. https://github.com/fchollet/keras, 2015.
- [7] Jeffrey Dalton, Laura Dietz, and James Allan. Entity query feature expansion using knowledge base links. In *Proceedings of the 37th international ACM SIGIR conference on Research & development in information retrieval*, pages 365–374. ACM, 2014.
- [8] Gerben Klaas Dirk de Vries and Steven de Rooij. Substructure counting graph kernels for machine learning from rdf data. Web Semantics: Science, Services and Agents on the World Wide Web, 35:71–84, 2015.
- [9] Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional neural networks on graphs with fast localized spectral filtering. In *Advances in neural information processing systems (NIPS)*, 2016.
- [10] Li Dong, Furu Wei, Ming Zhou, and Ke Xu. Question answering over freebase with multi-column convolutional neural networks. In *Proceedings of the 53rd Annual Meeting of the Association for Computational Linguistics*, pages 260–269. Association for Computational Linguistics, 2015.
- [11] David K. Duvenaud, Dougal Maclaurin, Jorge Iparraguirre, Rafael Bombarell, Timothy Hirzel, Alán Aspuru-Guzik, and Ryan P. Adams. Convolutional networks on graphs for learning molecular fingerprints. In *Advances in neural information processing systems (NIPS)*, pages 2224–2232, 2015.
- [12] Alberto Garcia-Duran, Antoine Bordes, and Nicolas Usunier. *Composing relationships with translations*. PhD thesis, CNRS, Heudiasyc, 2015.
- [13] Marco Gori, Gabriele Monfardini, and Franco Scarselli. A new model for learning in graph domains. In Proceedings. 2005 IEEE International Joint Conference on Neural Networks., volume 2, pages 729–734. IEEE, 2005.
- [14] Kelvin Guu, John Miller, and Percy Liang. Traversing knowledge graphs in vector space. arXiv preprint arXiv:1506.01094, 2015.
- [15] Frank L Hitchcock. The expression of a tensor or a polyadic as a sum of products. *Studies in Applied Mathematics*, 6(1-4):164–189, 1927.
- [16] Ben Hixon, Peter Clark, and Hannaneh Hajishirzi. Learning knowledge graphs for question answering through conversational dialog. In *Proceedings of NAACL HLT*, pages 851–861. Association for Computational Linguistics, 2015.
- [17] Diederik Kingma and Jimmy Ba. Adam: A method for stochastic optimization. arXiv preprint arXiv:1412.6980, 2014.
- [18] Thomas N. Kipf and Max Welling. Variational graph auto-encoders. arXiv preprint arXiv:1611.07308, 2016.
- [19] Thomas N. Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. In *International Conference on Learning Representations (ICLR)*, 2017.
- [20] Tamara G Kolda and Brett W Bader. Tensor decompositions and applications. SIAM review, 51(3):455–500, 2009.

- [21] Alexander Kotov and ChengXiang Zhai. Tapping into knowledge base for concept feedback: leveraging conceptnet to improve search results for difficult queries. In *Proceedings of the fifth ACM international conference on Web search and data mining*, pages 403–412. ACM, 2012.
- [22] Yujia Li, Daniel Tarlow, Marc Brockschmidt, and Richard Zemel. Gated graph sequence neural networks. In *International Conference on Learning Representations (ICLR)*, 2016.
- [23] Yankai Lin, Zhiyuan Liu, Huanbo Luan, Maosong Sun, Siwei Rao, and Song Liu. Modeling relation paths for representation learning of knowledge bases. arXiv preprint arXiv:1506.00379, 2015.
- [24] Tomas Mikolov, Ilya Sutskever, Kai Chen, Greg S Corrado, and Jeff Dean. Distributed representations of words and phrases and their compositionality. In Advances in neural information processing systems, pages 3111–3119, 2013.
- [25] Arvind Neelakantan, Benjamin Roth, and Andrew McCallum. Compositional vector space models for knowledge base completion. *arXiv preprint arXiv:1504.06662*, 2015.
- [26] Maximilian Nickel, Lorenzo Rosasco, and Tomaso Poggio. Holographic embeddings of knowledge graphs. arXiv preprint arXiv:1510.04935, 2015.
- [27] Maximilian Nickel, Volker Tresp, and Hans-Peter Kriegel. A three-way model for collective learning on multi-relational data. In *Proceedings of the 28th international conference on machine learning (ICML-11)*, pages 809–816, 2011.
- [28] Heiko Paulheim and Johannes Fümkranz. Unsupervised generation of data mining features from linked open data. In *Proceedings of the 2nd international conference on web intelligence, mining and semantics*, page 31. ACM, 2012.
- [29] Trang Pham, Truyen Tran, Dinh Phung, and Svetha Venkatesh. Column networks for collective classification. In AAAI, 2017.
- [30] Petar Ristoski, Gerben Klaas Dirk de Vries, and Heiko Paulheim. A collection of benchmark datasets for systematic evaluations of machine learning on the semantic web. In *International Semantic Web Conference*, pages 186–194. Springer, 2016.
- [31] Petar Ristoski and Heiko Paulheim. Rdf2vec: Rdf graph embeddings for data mining. In *International Semantic Web Conference*, pages 498–514. Springer, 2016.
- [32] Franco Scarselli, Marco Gori, Ah Chung Tsoi, Markus Hagenbuchner, and Gabriele Monfardini. The graph neural network model. *IEEE Transactions on Neural Networks*, 20(1):61–80, 2009.
- [33] Dominic Seyler, Mohamed Yahya, and Klaus Berberich. Generating quiz questions from knowledge graphs. In *Proceedings of the 24th International Conference on World Wide Web*, pages 113–114. ACM, 2015.
- [34] Richard Socher, Danqi Chen, Christopher D Manning, and Andrew Ng. Reasoning with neural tensor networks for knowledge base completion. In *Advances in neural information processing systems*, pages 926–934, 2013.
- [35] Theano Development Team. Theano: A Python framework for fast computation of mathematical expressions. arXiv e-prints, abs/1605.02688, 2016.
- [36] Kristina Toutanova, Victoria Lin, Wen-tau Yih, Hoifung Poon, and Chris 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, pages 1434–1444, Berlin, Germany, 2016.
- [37] Théo Trouillon, Johannes Welbl, Sebastian Riedel, Eric Gaussier, and Guillaume Bouchard. Complex embeddings for simple link prediction. In *Proceedings of the 33rd International Conference on Machine Learning*, pages 2071–2080, 2016.
- [38] Chenyan Xiong and Jamie Callan. Esdrank: Connecting query and documents through external semistructured data. In *Proceedings of the 24th ACM International on Conference on Information and Knowledge Management*, pages 951–960. ACM, 2015.
- [39] Chenyan Xiong and Jamie Callan. Query expansion with freebase. In *Proceedings of the 2015 International Conference on The Theory of Information Retrieval*, pages 111–120. ACM, 2015.
- [40] Bishan Yang, Wen-tau Yih, Xiaodong He, Jianfeng Gao, and Li Deng. Embedding entities and relations for learning and inference in knowledge bases. *arXiv* preprint arXiv:1412.6575, 2014.
- [41] Xuchen Yao and Benjamin Van Durme. Information extraction over structured data: Question answering with freebase. In *Proceedings of the 52nd Annual Meeting of the Association for Computational Linguistics*. Association for Computational Linguistics, 2014.