

If there's somethin' strange in you neighbourhood, who you gonna call?

On embeddings as an alternative paradigm for relational learning

Sebastijan Dumančić

Dept. of Computer Science
KU Leuven, Belgium

sebastijan.dumancic@cs.kuleuven.be

Alberto García-Durán and Mathias Niepert

NEC Labs Europe
Heidelberg, Germany

{alberto.duran,mathias.niepert}@neclab.eu

Abstract

Many real-world domains can be expressed as graphs and, more generally, as multi-relational knowledge graphs. Though reasoning and learning with knowledge graphs has traditionally been addressed by symbolic approaches, recent methods in (deep) representation learning has shown promising results for specialized tasks such as knowledge base completion. These approaches abandon the traditional symbolic paradigm by replacing symbols with vectors in Euclidean space. With few exceptions, symbolic and distributional approaches are explored in different communities and little is known about their respective strengths and weaknesses. In this work, we compare representation learning and relational learning on various relational classification and clustering tasks, and analyse the complexity of the rules used implicitly by these approaches. Preliminary results reveal possible indicators that could help in choosing one approach over the other for particular knowledge graphs.

Introduction

Learning from complex relational domains, where data contains instances and their mutual relationships, has typically been the focus of logic and graph-based machine learning methods. *Statistical relational learning* (SRL) (Getoor and Taskar 2007; de Raedt et al. 2016) uses the representational and reasoning framework of first-order logic to compactly represent such data, and combines it with probabilistic graphical models to facilitate reasoning under uncertainty. As first-order logic is a very general representation language, it serves as a unifying representational framework for many tasks such as classification, clustering, link prediction, and probabilistic modelling. *Graph mining* (GM) approaches (Chakrabarti and Faloutsos 2006) approach relational data as graph-structured data.

Representation learning for relational data has shown promising results for specific relational tasks such as knowledge base completion (Nickel et al. 2016). Knowledge graph embedding (KGE) methods take a radically different approach from the symbolic methods, and aim to represent instances and their relationship as vectors and/or matrices in the Euclidean space. Intuitively, KGEs introduce a novel view on relational propositionalization (Kramer, Lavrač, and

Flach 2001). The hope is that the geometry of the embedding space would resemble the structure of the data by, for example, keeping the instances participating in the same relationships close in the Euclidean space. This in turn allows one to apply standard propositional machine learning tools and retain their scalability, while at the same time preserving certain properties of structured relational data. These methods have proven to be very effective for the task of knowledge graph completion, where the goal is to identify missing links in the existing knowledge graph. They have also proven to be scalable to very large knowledge graphs.

Motivated by the success of KGE methods, there has been some recent work on combining more traditional logic-based SRL with representation learning methods. Šourek et al. (2018) introduce a relational extensions of neural networks (NN) by developing a template language for constructing neural networks from logical rules and data. Kazemi and Poole (2018) take a different view on relational NNs by means of the the relational logistic regression (Kazemi et al. 2014). Dumančić and Blockeel (2017) introduced a task-agnostic relational latent feature learning pipeline based on clustering that can be combined with any relational learner.

Unfortunately, these research directions have largely been developed in isolation and little understanding is currently available on the relative advantages of the respective approaches. Not only do they focus on different tasks but also different evaluation metrics. KGE methods, also referred to as *latent feature models*, typically focus on knowledge graph completion which requires very simple forms of relational reasoning. The evaluation metrics are often measuring the quality of rankings generated by the respective scoring functions. SRL methods, also referred to as *observed feature models*, typically focus on learning from small relational data, employing more complex forms of logical reasoning.

The focus of these methods already outlines the basic understanding of their limitations. A major advantage KGE methods is their scalability – they easily operate on knowledge graphs with millions of facts and thousands of relations. The main drawbacks of KGE methods are the black-box nature, limited reasoning on local information, and the difficulty of handling unseen instances. SRL methods are capable of capturing very complex relational patterns, are interpretable, and generalize beyond seen data. Unfortunately,

both inference and learning in SRL is highly complex, limiting its applicability.

In this work, we systematically compare KGE and logic-based SRL methods on standard relational classification and clustering tasks. We hope this contributes to a better understanding of their relative strengths and weaknesses. We focus on standard relational data sets as they offer more variety of tasks and reasoning complexity. We include both quantitative, in terms of performance, and qualitative analysis, in terms of extracted patterns of reasoning, in order to gain more insights into the suitability of these different methods.

Background and Related work

Knowledge graph embeddings Knowledge graph embeddings have emerged as an alternative paradigm for learning and reasoning with structured relational data. They replace symbols, i.e. instances and their relation predicates, with vectors and matrices in Euclidean space. That way the reasoning is performed through algebraic manipulations instead of more costly logical inference. The underlying idea of KGE methods is to associate a score with atoms in a database. Learning then consists of finding the vector representation of instances and their relations by maximizing (minimizing) the scores of the atoms in the database and minimizing (maximizing) the score of atoms not in the database. Two prototypical examples are:

- **TransE** (Bordes et al. 2013) which interprets relations as translations between instances in the Euclidean space. For each atom $r(h, t)$, r being a relation and h and t *head* and *tail* instances respectively, the score equals

$$s(r, h, t) = -||\mathbf{e}_h + \mathbf{e}_r - \mathbf{e}_t||,$$

i.e., the vector representation \mathbf{e}_h of a *head* instance translated by the relation vector \mathbf{e}_r should be close to the vector representation \mathbf{e}_t *tail* instance

- **DistMult** (Yang et al. 2015) which focuses on pairwise interactions of *latent* features with the following score

$$s(r, h, t) = (\mathbf{e}_h \circ \mathbf{e}_r) \mathbf{e}_t^T$$

where \circ is an element-wise product.

Checking the validity/truthfulness of any fact comes down to evaluating its score. The majority of KGE methods proposed so far (Wang et al. 2017) are a variation on the above scoring functions.

Comparing KGEs and logic-based SRL Understanding of advantages and disadvantages of KGE and logic-based SRL methods is currently very limited. Nickel, Jiang, and Tresp (2014) show that including both observable patterns, in form of random walks over a knowledge graph, and latent features from KGEs can greatly increase their performance and reduce the learning complexity. Pujara, Augustine, and Getoor (2017) show that KGEs have difficulties handling data with high degree of sparsity and noise – which is the case with every automatically created knowledge graph. Finally, Vig et al. (2018) show that KGE could be beneficial when the background knowledge about the task at hand is

Table 1: Dataset properties summarize the number of target and all instances, the number of attributes, and the number of relation types.

Dataset	Instances		Attributes		Relations	
	Target	Total	Target	Total	Target	Total
Hepa	500	5919	2	12	3	3
Muta	230	6124	3	7	3	7in
Terror	1293	1293	104	104	2	2
WebKB	920	3880	763	1207	4	5

limited, but if such knowledge is available then the SRL methods are preferable. Grefenstette (2013) introduces a formula framework for simulating logical reasoning through tensor calculation.

Methodology

The main goal of this study is to identify the strengths and weaknesses of KGE and logic-based SRL approaches to learning and reasoning with relational data. Concretely, we focus on the following questions:

- Q1** *Are KGEs a viable alternative to logic-based methods for relational classification?*
- Q2** *Are KGEs a viable alternative for relational clustering methods?*

More specifically, we focus on the following tasks:

- T1** Given a set of *target instances* (entities in a knowledge base), learn a model that predicts the value of the labels associated with those instances. We consider fully relational models learning the logical theory for predicting the labels, and a feature based models learning from the vector representation of target instances.
- T2** Given a set of instances of a specific type or domain, group them into a pre-specified number of groups. We consider methods operating on logical representation of data as well as those operating on the vector representation of instances.

Furthermore, we compare the two approaches across various tasks in order to *determine under which conditions KGEs are preferable to logic-based SRL methods and vice versa*. Given that KGEs are sensitive to the hyper-parameters, especially the size of the embeddings, we investigate the magnitude of those effects. Sensitivity to the hyper-parameter setup is less of a concern for classification tasks where one can use labels to tune the hyper-parameters. However, it poses a major issue for clustering tasks where no labels exists and there are no clear-cut performance criteria. A potential option would be to rely on certain geometric measures. These are, however, often based on various assumptions of limited generality and do not offer a performance measure such as classification accuracy (Estivill-Castro 2002).

Data We take standard relational learning data sets and use the available labels as ground truth for both classification and clustering. The IMDB data set is a snapshot of the Internet Movie Database, describing a set of movies with their actors and directors. The task is to distinguish between actors and directors. The UWCSE data set describes the employees of the University of Washington, their roles, publications, and courses. The task is to distinguish between students and professors. The Mutagenesis data set consists of a set of molecules and their structures, with the goal of predicting whether a compound is mutagenic or not. The WebKB dataset describes web pages of four US universities and their corresponding link structure. The pages are classified into seven groups according to their roles such as personal, departmental or project page. The Terrorists data set contains a network of terrorist attacks, each assigned to one of the 6 types of attacks. Finally, the Hepatitis data set describes a set of patients with a diagnosis of Hepatitis B and C. We intentionally focus on standard relational learning data sets because they typically expose more variety of reasoning: required reasoning ranges from attribute-only reasoning to multi-hop reasoning. Some of the properties are listed in Table 1. For each property, we differentiate between target instances – instances which contain labels, and the rest. This gives us a better opportunity to detect the conditions under which either of the respective approaches is preferable. In contrast, standard KB completion data sets are often very simple and only simple path-type rules are required to achieve a reasonable performance. Therefore, the only disadvantage of standard relational methods is that they might be very inefficient because of the data set size.

Classification Experiments We perform standard nested cross-validation. For each split the training data is used to learn the models and tune their parameters (using an inner cross-validation loop) and the unseen fold is used for testing. We report the performance in terms of accuracy as an average over individual splits. The labels were excluded from the data when learning the KGEs and considered only during the training of the classifier.

Clustering Experiments For the clustering experiments, we cluster the entire data set at once using the number of distinct labels as the number of clusters. Once the clustering is obtained, we compare it to the ground truth determined by the class labels using the adjusted Rand index (Rand 1971) as evaluation measure. We use Spectral (Ng, Jordan, and Weiss 2001) and Hierarchical (Ward 1963) clustering algorithms and compare embedding-based clustering with state-of-the-art relational clustering method ReCeNT (Dumančić and Blockeel 2017). ReCeNT defines a very flexible similarity measure for relational objects which is used in the conjunction with the

Knowledge Graph Embeddings Many KGEs exist in the literature (Wang et al. 2017). We decide to focus on two prototypical and commonly used instances:

TransE and DistMult. We evaluate the dimensions in $\{10, 20, 30, 50, 80, 100\}$ and train for 100 epochs.

As KGE methods are focused on the knowledge graph completion task, they assume that all instances are given at once and focus on filling in the missing links in data. Therefore, they have difficulties with unseen instances. We do not address this issue here, but simply learn the representation of both training and test data at the same time (with labels excluded).

Relational Learning We currently limit the analysis to Inductive logic programming (ILP) methods (Raedt 2008) and ignore the probabilistic aspect of SRL methods. This is solely due to better predictive rule induction support of ILP. For that reason, we decide to use the relational decision tree learner TILDE (Blockeel and De Raedt 1998) as a relational baseline. We report results of two TILDE variants: one trained on the original (logical) data representation (termed TILDE), and the one trained on the *relational* latent features created by CUR²LED (Dumančić and Blockeel 2017) (termed TILDE-latent). CUR²LED creates latent features that remain in the logical representation (i.e., are expressed through predicate logic) and should not be confused with the vector representation based latent features.

Classification Results

We first focus on comparing the classifiers with the same learning bias, namely propositional and relational decision trees (DT), as this constitutes the fairest comparison. The results (Figure 1) show that the decision tree trained on the embedding features outperforms TILDE only on the Hepatitis data set. However, it does not outperform TILDE-latent on any data set. The performance is similar only on the Terrorists data set. This implicates that relational learners are able to capture certain information that embeddings likely do not contain. Moreover, fully acknowledging relational information (especially distinguishing between attributes of instances and their mutual relationships) while learning the latent representation (Dumančić and Blockeel 2017) seems beneficial as TILDE-latent outperforms TILDE in all but one case. An important aspect to keep in mind is that KGE methods see both training and test data at training time. This gives them a certain advantage and the question is to what extent this affects the performance. We did not observe significant difference between TransE and DistMult.

The classifiers with non-linear decision function, non-linear SVM and kNN, perform substantially better than the decision tree with the embedding features. Even though both SVM and kNN are able to capture more complex feature interactions than a decision tree, the results indicate that their results are not significantly better than those of the relational methods. SVM strongly outperforms TILDE on the Hepatitis dataset, both are similar in performance of the Mutagenesis and Terrorists dataset while TILDE performs much better on the WebKB dataset. kNN slightly outperforms TILDE on the Hepatitis, performs slightly worse than TILDE on Mutagenesis and Terrorists, and substantially worse on the WebKB data set. TILDE-latent outperforms SVM and kNN on

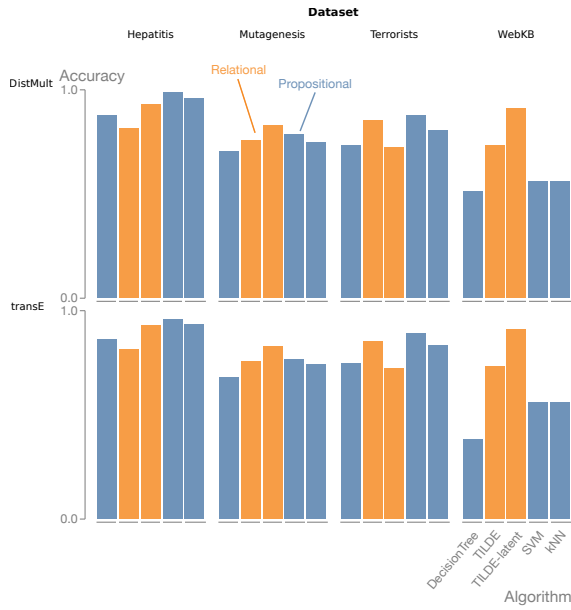


Figure 1: Classification performance. Individual rows contain results with distinct KGE methods. The color indicates whether the learning is propositional or relational. The performance of TILDE variants is simply duplicated on two graphs, for easier comparison.

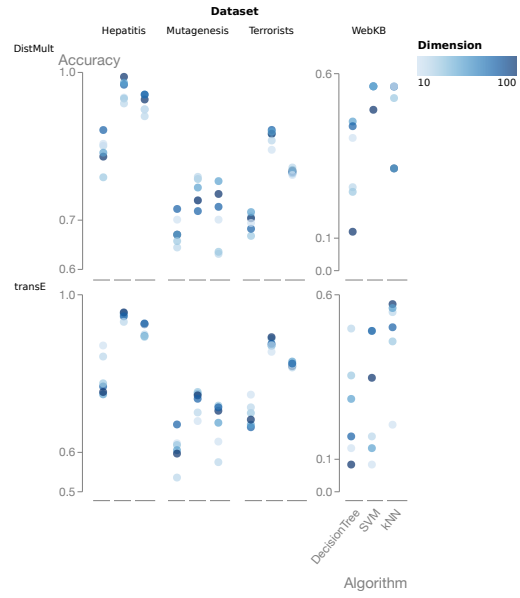


Figure 2: Performance of KGEs varies substantially with the dimension. The rows show performance of the KGE methods, while the brightness indicates the dimension. (WebKB has a separate scale because the performance is in a very different range compared to other datasets)

Table 2: Properties of extracted rules are summarized as a proportion of relation and attribute predicates they contain. *Rule properties* section describes the proportion of rules that contain *relation* predicates only, *attribute* predicates only and the mix of both, for each dataset. *Dataset properties* section shows the proportion of possible attribute and relation predicates that are used in the extracted rules. For example, the rules on the Hepatitis dataset use 100 % of the possible attribute predicates, and 66 % of relation predicates. *Neighbourhood* refers to the proportion of attribute and relation predicates of the non-target instances for which a direct link with target instances exists.

Dataset	Reasoning depth	Rule properties			Dataset properties		
		Relations	Attributes	Mix	Attributes	Relations	Neighbourhood
Hepatitis	1.4	10 %	38 %	52 %	100 %	66 %	70 %
Terrorists	1	0 %	95 %	5 %	35 %	100 %	0 %
Mutagenesis	0	0 %	100 %	0 %	100 %	0 %	0 %
WebKB	2	5 %	76 %	19 %	4 %	50 %	1 %

the Mutagenesis and WebKB data, is much closer in performance to SVM and kNN of the Hepatitis but struggles with the Terrorists. These results suggest that the ability to capture more complex dependencies allows SVM and kNN to compensate for the lack of the explicit relational information. This also suggests that then labelled instance are not linearly separable in the embedding space, which explain why both SVM and kNN perform much better than DTs.

Analyzing these results with respect to the semantics of the predicates used in the extracted rules yields further interesting results. More precisely, we differentiate between *attribute predicates* that associate a specific value of an attribute with an instance, and *relation predicates* that connect two instances. We further distinguish between *target* instances having an associated label, and *neighbourhood*

instances that provide additional data. Properties of rules learned by TILDE (Table 2) suggest that KGE have an edge over the SRL methods when most of the information in the neighbourhood of instances is relevant. For example, on the Hepatitis data set the induced rules incorporate 100 % of the target attributes and 66 % of relations involving target instances, as well as 70 % of the predicates related to the neighbouring instances. This also holds for the Terrorists data; though 35 % does not constitutes 'most of the information in the neighbourhood', we have found that many of the attributes are highly correlated and thus the number of predictive attributes is effectively higher.

The remaining two data sets are different in the sense that only a fraction of information is found predictive. On

the Mutagenesis data set¹, even though all the attributes of molecules are found predictive, none of the relations were found predictive and thus none of the information about atoms they contain. Thus, only a fraction of available information is used. On the WebKB data set only 4 % of the attributes have been found predictive, as well as 50 % of relations. An explanation for such a big difference in performance might be that SRL methods have to select few predictive rules while learning theories, and thus can discard irrelevant information. In contrast, the learning principle of KGEs is designed to take all of the information into account, which seems to make them underperform.

Figure 2 show the differences in performances when the dimension of the embeddings is changed. These results indicate the importance of choosing the embedding dimension, as the performance varies substantially with the dimension. That is especially true for the Mutagenesis and WebKB datasets. Unfortunately, there does not seem to be a general rules how to choose the dimension: higher does not lead to better results. Fortunately, this is not a major issue for the classification tasks as the dimension can be treated as a parameter to tune.

Clustering results

The first issue when using KGEs for entity clustering is which distance or similarity measure to use. Even though KGEs embed instances in Euclidean space, that space is usually high-dimensional and, thus, simple Euclidean distance is likely not to be informative. Therefore, to better understand how to use KGEs for clustering, we first survey the possible distance and similarity measures. We focus on the measure available in the `sci-kit learn` package (Pedregosa et al. 2011) in combination with Spectral and Hierarchical clustering.

We first use every distance and similarity measure available to perform clustering for each of the dimensions in {10, 30, 50, 80, 100}. Within each dimension, we rank the measure according to their performance per dataset and report average rank per dimension. The ranks for the five best performing ones are reported in Table 3 for Spectral clustering and in Table 4 for Hierarchical clustering.

These results suggest that clustering with KGE is not straightforward as there is no single measure that is an obvious winner. Polynomial kernel seems to be the overall winner with spectral clustering, but it is mostly the second best measure to use on the individual data set. The results with hierarchical clustering show even greater variance: cosine and correlation distances seem to be an overall winner but they average ranks spread between 4 and 6. This means that a different distance/similarity measure is the most appropriate one for each data set, but at the same time it performs bad with different data set and embeddings dimension. Therefore, a major challenge with using KGEs as a means for relational clustering is the choice of the right distance or similarity, but unfortunately clustering settings does not provide

¹we use the version of the data set without any rings structures and additional background knowledge which is difficult to incorporate in KGE methods

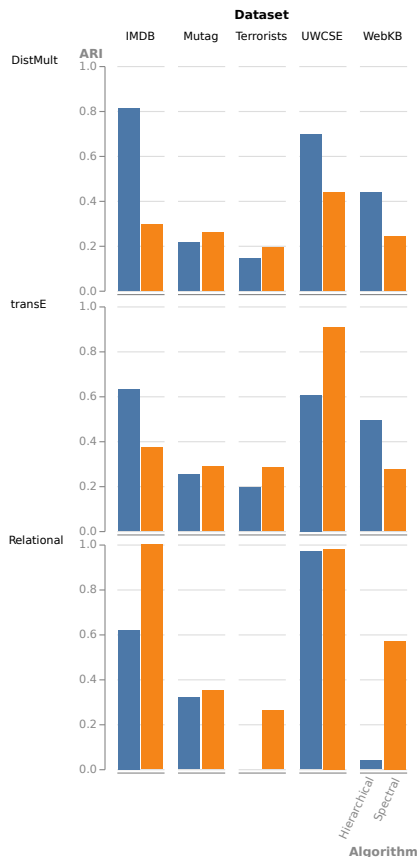


Figure 3: Clustering performance per dataset. The first two rows correspond to distinct KGE methods, while the third one contains results of the relational clustering approach.

a ground truth that can be used to find the most suitable measure. In further experiments, we use cosine and polynomial distance.

Comparing the performance of clustering approaches yields mixed results (Figure 3). For instance, on the IMDB data set embeddings do better than the relational methods with Hierarchical clustering, while the relational methods substantially outperforms KGEs with Spectral clustering. Similar holds for the Terrorists and WebKB data. However, on the Mutagenesis and UWCSE data sets, relational methods do better in both cases. With an exception in the Terrorists data, the best overall result is achieved by the relational learning approach. It is interesting to note that these are the same data sets where relational methods have the advantage in the classification settings. It is also interesting to note that, while relational clustering method seems to achieve better results with Spectral clustering, the performance of clustering algorithms is more balanced in the case of KGEs. This implies that the KGEs introduce *smoother* geometry that is more accessible to wider class of clustering algorithms, but more elaborate experiments are needed to confirm this.

Unfortunately, using KGEs for clustering seems to be highly sensitive to the choice of dimension (Figure 4). Sim-

Table 3: Ranking of similarity measure for Spectral clustering. Table 4: Rankings of distances for Hierarchical clustering.

Embed	Measure	Dimension					Avg
		10	30	50	80	100	
transE	polynomial	2.2	2.4	2.2	2.0	2.2	2.23
	sigmoid	2.8	3.6	3.2	2.4	3.2	3.0
	rbf	3.0	2.6	3.6	3.2	3.0	3.03
	laplace	4.0	3.0	3.3	3.4	3.4	3.33
	NN	3.0	3.8	3.6	3.2	3.6	3.4
distMult	polynomial	3.2	1.6	1.6	1.6	1.4	1.9
	rbf	2.4	2.8	3.2	3.0	3.6	2.83
	sigmoid	2.6	3.0	2.6	2.4	2.8	2.9
	NN	3.6	3.4	3.8	3.4	3.0	3.53
	laplacian	3.2	4.2	3.8	4.6	4.2	3.83

Embed	Measure	Dimension					Avg
		10	30	50	80	100	
transE	cosine	3.8	6.0	3.8	3.8	4.4	4.43
	correlation	6.8	4.2	8.4	4.2	4.0	5.5
	braycurtis	8.4	5.2	4.6	4.2	8.4	6.37
	canberra	7.2	9.2	9.4	5.2	5.2	7.9
	chebysev	6.0	13.0	13.2	9.8	10.0	9.73
distMult	correlation	6.0	3.8	8.0	2.0	7.4	5.87
	cosine	8.8	8.0	2.2	5.4	8.2	6.7
	braycurtis	7.2	8.8	5.8	2.6	5.8	6.83
	l1	6.2	7.4	9.2	11.8	7.2	8.0
	canberra	11.0	10.6	5.6	4.2	6.2	8.27

ply altering the dimension varies the results from a completely random clustering ($ARI \approx 0$), to the best obtained one. As finding the means to somehow choose the correct value directly from the data is very difficult for clustering, this severely limits the applicability of KGEs for clustering tasks.

Conclusions and Future Work

The most important takeaway messages from this work are the following:

- **KGE seems to be suitable for curated data** KGEs seem to have difficulties in the case when only a small fraction of available information is necessary for the given prediction task. SRL methods do not have that issue as they cherry pick useful information during the learning phase. This observation explains why KGEs perform well on the knowledge base completion task where the complexity of reasoning is low, but the dataset is huge. This further indicates the target use cases for the respective approaches: KGEs target simple relational reasoning with huge amounts of data, while SRL targets complex reasoning tasks with not a lot of data.
- **KGE might be useful for relational clustering but needs further research** Although logic-based relational clustering algorithms achieve the overall best results, clustering instances in the embeddings space does not lack much behind. They certainly show potential for this task, however they rise many problem, such as the question of an appropriate distance/similarity measure.
- **Hyper-parameters matter a lot** A major disadvantage of KGEs is their sensitivity to hyper-parameters. Our experiments show there is no clear strategy for choosing the right dimension. Though this might be less of an issue for classification problems, it poses a major one for clustering where there is no option to tune the parameters.

Besides the above outlined point, some obvious (dis)advantages are worth re-iterating here. A strong advantage of KGEs is their scalability, at the expense of their black-box nature and limited reasoning capabilities. SRL

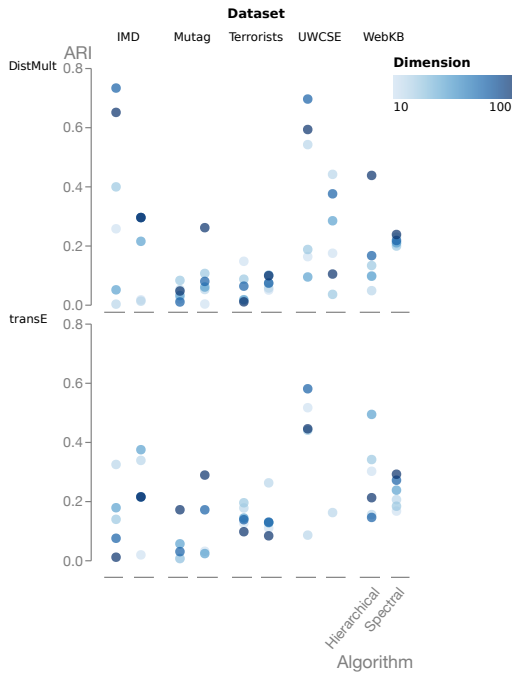


Figure 4: The performance of clustering method varies substantially with dimension (indicated by the brightness).

methods are a direct opposite – they can capture very complex reasoning, are interpretable but currently of a limited scalability.

The analysis presented here is still preliminary and has to be extended in several ways. We plan to extend this study in three main directions. First, adding more datasets is necessary to confirm the preliminary results. Second, including a larger variety of relational learners is necessary to get a complete picture. Currently we considered only TILDE as the relational baseline, which was often outperformed by SVM and kNN trained on the embeddings of entities. Therefore, a fairer comparison would be to compare embedding-based SVM and kNN with relational learners with similar non-linear decision functions such as kFOIL (Landwehr et al. 2006), nFOIL (Landwehr, Kersting, and De Raedt 2005) and kNN with relational similarity measures (Dumančić and Blockeel 2017; Shervashidze et al. 2011). Third, we focus here on the prototypical KGE methods of TransE and DistMult and including other state-of-the-art KGE methods, such as ComplEx (Trouillon et al. 2016) and ConvE (Dettmers et al. 2018), is worthwhile (though the performance is likely to be very similar (Kadlec, Bajgar, and Kleindienst 2017)).

Additionally, a careful inspection of the scalability of SRL methods on the standard KGE knowledge graph might be interesting. Though SRL methods are in principle less scalable than the KGEs, one might overcome that by limiting the expressivity of SRL methods by limiting the length of clauses. Such a restriction might not have a big impact on the performance for standard KGE tasks, but might largely increase the scalability.

As a final note, this work does not aim to critique the KGEs, but should serve as point for new research directions combining the strengths of the two respective approaches. There is obviously a need to integrate them, and several approaches already explore this line of work (Minervini et al. 2017; Demeester, Rocktäschel, and Riedel 2016; Schlichtkrull et al. 2017). However, all of the existing approaches focus on incorporating certain logical concepts into KGEs. This unfortunately uses little of the power of first-order logic while retaining all of the disadvantages of KGEs.

Conclusion

Many problem nowadays are naturally expressed in form of relational and graph structures data. This includes social and protein interaction networks, biological data, knowledge graphs and many more. Two main machine learning paradigms for analysing such data, knowledge graphs embeddings and statistical relational learning, have mostly been studied in isolation so far. This work is the first, to the best of our knowledge, that systematically compares these two paradigms on the standard machine learning tasks – classification and clustering. Our preliminary results indicate that knowledge graph embeddings are suitable when data is *curated* – when only the *relevant* information is preserved in the data, while the major strength of the statistical relational learning methods is their ability to select relevant information during training. Embedding methods also show certain potential relational clustering, but also raise issues due to

their sensitivity to the hyper-parameter choice. We hope this work inspires new research directions focused on combining the strengths of both approaches.

References

- Blockeel, H., and De Raedt, L. 1998. Top-down induction of first-order logical decision trees. *Artificial Intelligence* 101(1–2):285 – 297.
- Bordes, A.; Usunier, N.; Garcia-Duran, A.; Weston, J.; and Yakhnenko, O. 2013. Translating embeddings for modeling multi-relational data. In Burges, C. J. C.; Bottou, L.; Welling, M.; Ghahramani, Z.; and Weinberger, K. Q., eds., *Advances in Neural Information Processing Systems* 26. Curran Associates, Inc. 2787–2795.
- Chakrabarti, D., and Faloutsos, C. 2006. Graph mining: Laws, generators, and algorithms. *ACM Comput. Surv.* 38(1).
- de Raedt, L.; Poole, D.; Kersting, K.; and Natarajan, S. 2016. *Statistical Relational Artificial Intelligence: Logic, Probability, and Computation*. Morgan & Claypool Publishers.
- Demeester, T.; Rocktäschel, T.; and Riedel, S. 2016. Lifted rule injection for relation embeddings. In *Proceedings of the 2016 Conference on Empirical Methods in Natural Language Processing, EMNLP 2016, Austin, Texas, USA, November 1-4, 2016*, 1389–1399.
- Dettmers, T.; Pasquale, M.; Pontus, S.; and Riedel, S. 2018. Convolutional 2d knowledge graph embeddings. In *Proceedings of the 32th AAAI Conference on Artificial Intelligence*.
- Dumančić, S., and Blockeel, H. 2017. An expressive dissimilarity measure for relational clustering using neighbourhood trees. *Machine Learning* 106(9):1523–1545.
- Dumančić, S., and Blockeel, H. 2017. Clustering-based relational unsupervised representation learning with an explicit distributed representation. In *Proceedings of the Twenty-Sixth International Joint Conference on Artificial Intelligence, IJCAI-17*, 1631–1637.
- Estivill-Castro, V. 2002. Why so many clustering algorithms: A position paper. *SIGKDD Explor. Newsl.* 4(1):65–75.
- Getoor, L., and Taskar, B. 2007. *Introduction to Statistical Relational Learning (Adaptive Computation and Machine Learning)*. The MIT Press.
- Grefenstette, E. 2013. Towards a formal distributional semantics: Simulating logical calculi with tensors. *Proceedings of the Second Joint Conference on Lexical and Computational Semantics*.
- Kadlec, R.; Bajgar, O.; and Kleindienst, J. 2017. Knowledge base completion: Baselines strike back. In *Proceedings of the 2nd Workshop on Representation Learning for NLP, Rep4NLP@ACL 2017, Vancouver, Canada, August 3, 2017*, 69–74.
- Kazemi, S. M., and Poole, D. 2018. Relnn: A deep neural model for relational learning. In *AAAI*.

- Kazemi, S. M.; Buchman, D.; Kersting, K.; Natarajan, S.; and Poole, D. 2014. Relational logistic regression.
- Kramer, S.; Lavrač, N.; and Flach, P. 2001. *Propositionalization Approaches to Relational Data Mining*. Berlin, Heidelberg: Springer Berlin Heidelberg. 262–291.
- Landwehr, N.; Passerini, A.; De Raedt, L.; and Frasconi, P. 2006. kfoil: Learning simple relational kernels. In *Proceedings of the 21st National Conference on Artificial Intelligence - Volume 1*, AAAI’06, 389–394. AAAI Press.
- Landwehr, N.; Kersting, K.; and De Raedt, L. 2005. nfoil: Integrating naïve bayes and foil. In *Proceedings of the 20th National Conference on Artificial Intelligence - Volume 2*, AAAI’05, 795–800. AAAI Press.
- Minervini, P.; Demeester, T.; Rocktäschel, T.; and Riedel, S. 2017. Adversarial sets for regularising neural link predictors. In *Proceedings of the Thirty-Third Conference on Uncertainty in Artificial Intelligence, UAI 2017, Sydney, Australia, August 11-15, 2017*.
- Ng, A. Y.; Jordan, M. I.; and Weiss, Y. 2001. On spectral clustering: Analysis and an algorithm. In *Advances in neural information processing systems*, 849–856. MIT Press.
- Nickel, M.; Murphy, K.; Tresp, V.; and Gabrilovich, E. 2016. A review of relational machine learning for knowledge graphs. *Proceedings of the IEEE* 104(1):11–33.
- Nickel, M.; Jiang, X.; and Tresp, V. 2014. Reducing the rank in relational factorization models by including observable patterns. In Ghahramani, Z.; Welling, M.; Cortes, C.; Lawrence, N. D.; and Weinberger, K. Q., eds., *Advances in Neural Information Processing Systems 27*. Curran Associates, Inc. 1179–1187.
- Pedregosa, F.; Varoquaux, G.; Gramfort, A.; Michel, V.; Thirion, B.; Grisel, O.; Blondel, M.; Prettenhofer, P.; Weiss, R.; Dubourg, V.; Vanderplas, J.; Passos, A.; Cournapeau, D.; Brucher, M.; Perrot, M.; and Duchesnay, E. 2011. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research* 12:2825–2830.
- Pujara, J.; Augustine, E.; and Getoor, L. 2017. Sparsity and noise: Where knowledge graph embeddings fall short. In *Conference on Empirical Methods in Natural Language Processing (EMNLP)*.
- Raedt, L. D. 2008. *Logical and Relational Learning: From ILP to MRDM (Cognitive Technologies)*. Berlin, Heidelberg: Springer-Verlag.
- Rand, W. M. 1971. Objective criteria for the evaluation of clustering methods. *Journal of the American Statistical Association* 66(336):846–850.
- Schlichtkrull, M. S.; Kipf, T. N.; Bloem, P.; van den Berg, R.; Titov, I.; and Welling, M. 2017. Modeling relational data with graph convolutional networks. *CoRR* abs/1703.06103.
- Shervashidze, N.; Schweitzer, P.; van Leeuwen, E. J.; Mehlhorn, K.; and Borgwardt, K. M. 2011. Weisfeiler-lehman graph kernels. *J. Mach. Learn. Res.* 12:2539–2561.
- Trouillon, T.; Welbl, J.; Riedel, S.; Gaussier, E.; and Bouchard, G. 2016. Complex embeddings for simple link prediction. In *International Conference on Machine Learning (ICML)*, volume 48, 2071–2080.
- Vig, L.; Srinivasan, A.; Bain, M.; and Verma, A. 2018. An investigation into the role of domain-knowledge on the use of embeddings. In Lachiche, N., and Vrain, C., eds., *Inductive Logic Programming*, 169–183. Cham: Springer International Publishing.
- Šourek, G.; Aschenbrenner, V.; Železny, F.; and Kuželka, O. 2018. Lifted relational neural networks: Efficient learning of latent relational structures.
- Wang, Q.; Mao, Z.; Wang, B.; and Guo, L. 2017. Knowledge graph embedding: A survey of approaches and applications. *IEEE Transactions on Knowledge and Data Engineering* 29(12):2724–2743.
- Ward, J. H. 1963. Hierarchical grouping to optimize an objective function. *Journal of the American Statistical Association* 58(301):236–244.
- Yang, B.; tau Yih, W.; He, X.; Gao, J.; and Deng, L. 2015. Embedding entities and relations for learning and inference in knowledge bases. In *International Conference on Learning Representations*.