

# An Evaluation of Hubness Reduction Methods for Entity Alignment with Knowledge Graph Embeddings

Daniel Obraczka<sup>a</sup> and Erhard Rahm<sup>b</sup>

ScaDS.AI/Database Group, Leipzig University, Germany

{obraczka, rahm}@informatik.uni-leipzig.de

**Keywords:** Hubness Reduction, Nearest Neighbor Search, Knowledge Graph Embedding, Entity Alignment.

**Abstract:** The heterogeneity of Knowledge Graphs is problematic for conventional data integration frameworks. A possible solution to this issue is using Knowledge Graph Embeddings (KGEs) to encode entities into a lower-dimensional embedding space. However, recent findings suggest that KGEs suffer from the so-called hubness phenomenon. A dataset that suffers from hubness has a few popular entities that are nearest neighbors of a highly disproportionate amount of other entities. Because the calculation of nearest neighbors is an integral part of entity alignment with KGEs, hubness reduces the accuracy of the matching result. We therefore investigate a variety of hubness reduction techniques and utilize approximate nearest neighbor (ANN) approaches to offset the increase in time complexity stemming from the hubness reduction. Our results suggest, that hubness reduction in combination with ANN techniques improves the quality of nearest neighbor results significantly compared to using no hubness reduction and exact nearest neighbor approaches. Furthermore, this advantage comes without losing the speed advantage of ANNs on large datasets.

## 1 INTRODUCTION

Knowledge Graphs (KGs) contain information in structured machine-readable form as triples (*subject, predicate, object*). Integrating multiple KGs is a necessary step for a plethora of downstream tasks such as question answering (Usbeck et al., 2019), recommender systems (Sun et al., 2020a) and many more. The heterogeneous nature of KGs poses a challenge to many data integration frameworks. In recent years Knowledge Graph Embeddings (KGEs) have seen a surge of attention from the research community as a possible solution to tackle the heterogeneous nature of this data structure (Ali et al., 2020; Sun et al., 2020b). While numerous models have been devised to obtain KGEs, little consideration has been given to refining their use in the alignment step of the data integration pipeline. A recent study (Sun et al., 2020b) has discovered, that KGEs suffer from a problem called *hubness*, which refers to an unequal distribution of *k*-nearest neighbors (kNN) between points. In data that suffers from hubness a few hubs are the kNN of a lot of data points, while many data points are the nearest

neighbors of no other points. Hubness can be found in many high-dimensional datasets (Feldbauer et al., 2018) and given the importance of kNN in a diverse range of tasks this finding has been determined as a problem in applications such as recommender systems (Hara et al., 2015a), speech recognition (Vincent et al., 2014), image classification (Tomašev and Buza, 2015) and many more. For a data integration setting where usually an entity only has one true match in another dataset hubness is detrimental for the alignment quality. To investigate the effects of hubness on data integration tasks we used 15 different Knowledge Graph Embedding approaches on 16 alignment tasks containing samples of KGs with varying properties. This procedure resulted in 240 KGEs as input for our study. We examine six different hubness reduction methods and six different (approximate) nearest neighbor algorithms with regards to accuracy and execution time.

The contributions of our work are as follows:

- We provide the first (to our knowledge) extensive evaluation of hubness reduction techniques for entity alignment with knowledge graph embeddings.
- The result of our work suggests, that using approximate nearest neighbor algorithms with hubness reduction improves kNN results for align-

<sup>a</sup>  <https://orcid.org/0000-0002-0366-9872>

<sup>b</sup>  <https://orcid.org/0000-0002-2665-1114>

ment significantly in terms of accuracy and for large datasets also with regards to execution time. We ensure the significance of our findings with statistical tests.

- We present the first framework for entity alignment, that makes a wide array of hubness reduction methods available <https://github.com/dobraczka/kiez>. Furthermore we make all our results and configurations freely available in a separate benchmarking repository <https://github.com/dobraczka/kiez-benchmarking>.

We start by giving an overview of related work, followed by a synopsis of hubness reduction for the problem of entity alignment in Section 3. Our extensive evaluation follows in Section 4 and we close with a conclusion.

## 2 RELATED WORK

We start by motivating the hubness problem and the related research. Subsequently, we present different methods to mitigate hubness. Finally, we give a brief overview over different KGE approaches.

### 2.1 Hubness

First noticed in music recommendation (Pachet and Aucouturier, 2004) the phenomenon of hubness has been shown to occur in high-dimensional data (Radovanovic et al., 2009). A facet of the so-called *curse of dimensionality* is that distances between all points in high-dimensional data become very similar. The reason for this *distance concentration*, is that with increasing dimensions the volume of a unit hypercube grows faster than the volume of a unit hyperball. Correspondingly, numerous distance metrics (e.g. the euclidean distance) lose their relative contrast, i.e. given a query point the distance between the nearest and farthest neighbor decreases almost entirely (Aggarwal et al., 2001). Related to nearest neighbors (NN) is the problem of *hubness*.

**Definition 1** (k-occurrence). *Given a non-empty dataset  $D \subseteq \mathbb{R}^m$  with  $n$  objects in an  $m$ -dimensional space. We can count how often an object  $x \in D$  occurs in the  $k$ -nearest neighbors of all other objects  $D \setminus x$ . This count is referred to as  $k$ -occurrence  $O^k(x)$ .*

Hubness now refers to the problem, that with increasing dimensionality the distribution of the  $k$ -occurrence is skewed to the right, which signifies the occurrence of *hubs*, i.e. "popular" nearest neighbors, that occur more frequently in  $k$ -NN lists than other

points (Feldbauer et al., 2018). The hubness phenomenon is not yet well understood. While some empirical results indicate, that hubness arises with high intrinsic dimensionality of the data (Radovanović et al., 2010), a later study suggests, that density gradients are the reason for hubness (Low et al., 2013). Density gradients are spatial variations in density in an area, in this case over an empirical data distribution (Feldbauer and Flexer, 2019).

### 2.2 Hubness Reduction

Several different approaches have been proposed to reduce hubness. Given two objects  $x$  and  $y$  the nearest neighbor relation between them is symmetric if  $x$  is a nearest neighbor of  $y$  and vice versa. Hubness leads to an asymmetry in NN relations, because hubs are NNs of many data points, while only one data point can be the nearest neighbor of a hub (Feldbauer and Flexer, 2019). One category of hubness reduction methods therefore tries to mend asymmetric relations by transforming these relations to secondary distance spaces from primary distance spaces (e.g. euclidean). While for example *mutual proximity* (Schnitzer et al., 2012) was developed specifically to reduce hubness, other methods such as *local scaling* (Zelnik-Manor and Perona, 2004) and the (*non-iterative*) *contextual dissimilarity measure* (Jégou et al., 2007) were later found to reduce hubness (Schnitzer et al., 2012). *Spatial centrality* refers to the fact, that objects closer to the mean of a data distributions are more likely to become hubs with increasing dimensionality (Radovanović et al., 2010). Accordingly, another category of hubness reduction techniques aims to reduce spatial centrality by subtracting the centroid of the data (Suzuki et al., 2013) or localized centering (Hara et al., 2015b). Subsequent works argue that variants of these centering approaches work in reducing hubness by flattening the density gradient (Hara et al., 2016). For a more comprehensive overview of hubness reduction techniques we refer to (Feldbauer et al., 2018; Feldbauer and Flexer, 2019). In Section 3.3 we will present a more detailed view of the mentioned approaches with regards to entity alignment.

### 2.3 Knowledge Graph Embedding

Knowledge Graph Embedding approaches aim to encode KG entities into a lower-dimensional space. This alleviates the heterogeneity present across different KGs and makes it usable for downstream machine learning tasks.

Translational models encode relations as translations from the embedding of the head entity to tail entity embedding. The pioneering approach TransE (Bordes et al., 2013) relies on the distance between  $\mathbf{h} + \mathbf{r}$  and  $\mathbf{t}$ , where  $\mathbf{h}, \mathbf{r}$  and  $\mathbf{t}$  are the respective embedding vectors of the head and tail entity  $h, t$  and the relation  $r$  of the triple  $(h, r, t)$ . TransE has problems modeling  $1 - n$  or  $n - n$  relations. To address this shortcoming several different methods were devised which encode relations in their own hyperplane (Wang et al., 2014) or even relation-specific spaces (Lin et al., 2015).

Another category of embedding approaches relies on tensor-factorization. RESCAL (Nickel et al., 2011) models a KG as a 3D binary tensor  $\mathcal{X} \in \mathbb{R}^{n \times n \times m}$  with  $n$  and  $m$  being the number of entities and relations respectively. Each relation therefore is a matrix  $W_r \in \mathbb{R}^{n \times n}$ , with the weights  $w_{i,j}$  capturing the interaction between the  $i$ -th latent factor of  $\mathbf{h}$  and  $j$ -th latent factor of  $\mathbf{t}$ . The plausibility of a triple  $(h, r, t)$  is therefore scored by

$$f(h, r, t) = \mathbf{h}^T \mathbf{W}_r \mathbf{t}. \quad (1)$$

Several methods (Sun et al., 2019; Nickel et al., 2016; Kazemi and Poole, 2018) build on this idea by using different scoring functions.

With the success of deep learning techniques in other fields, they were applied to KGEs as well. ConvE (Dettmers et al., 2018) relies on a set of 2-dimensional convolutional filters to capture interactions between  $\mathbf{h}$  and  $\mathbf{r}$ . The approach GCNAlign (Wang et al., 2018) uses attribute embeddings with graph convolutions to embed cross-lingual KG entities into a unified vector space.

Path-based approaches incorporate information of multi-hop neighbors of nodes. For example IP-TransE (Zhu et al., 2017) relies on an extension of TransE to incorporate multi-step paths.

## 2.4 Entity Alignment

Extensive research has been done to devise methods that aid in the matching of entities across different data sources. While most methodologies center around aligning tabular data (Christen, 2012), the field of collective entity resolution exploits relational information in the alignment process (Bhattacharya and Getoor, 2007). For example (Pershina et al., 2015) use Personalized PageRank to propagate similarities in their graph of potential matches. (Huang et al., 2020) utilize a human-in-the-loop approach to make high-quality alignments leveraging relational information.

A plethora of approaches have been devised to tackle entity alignment via KGE. These techniques

usually rely on a given *seed alignment* containing entity pairs, which are known to refer to the same real-world object. MultiKE learns entity embeddings by using different views for different aspects of an entity (Zhang et al., 2019). AttrE (Trisedya et al., 2019) relies on an attribute encoding function to encode the entity attributes of the different KGs into the same space. Both MultiKE and AttrE rely on a translational approach to encode relationship information.

For a more detailed overview over KGEs we refer the reader to these surveys (Ali et al., 2020; Dai et al., 2020). A synopsis and benchmarking study of KGE approaches that are used for entity alignment can be found in (Sun et al., 2020b). This study also discovered, that KGEs suffer from hubness. However, to our knowledge, no systematic study on hubness reduction methods for entity alignment with knowledge graph embeddings has been published.

## 3 HUBNESS REDUCTION FOR ENTITY ALIGNMENT

In the following, we illustrate the task of entity alignment, present ways to measure hubness and provide some details of our framework and the hubness reduction methods we implemented for the use case of entity alignment. Finally, we give an overview of the approximate nearest neighbor approaches we utilize.

### 3.1 Entity Alignment

For our purposes a KG is a tuple  $\mathcal{KG} = (\mathcal{E}, \mathcal{P}, \mathcal{L}, \mathcal{T})$ , where  $\mathcal{E}$  is the set of entities,  $\mathcal{P}$  the set of properties,  $\mathcal{L}$  the set of literals and  $\mathcal{T}$  the set of triples. KGs consist of triples  $(h, r, t) \in \mathcal{T}$ , with  $h \in \mathcal{E}$ ,  $r \in \mathcal{P}$  and  $t \in \{\mathcal{E}, \mathcal{L}\}$ . Given two KGs the goal of entity alignment lies in finding the mapping  $\mathcal{M} = \{(e_1, e_2) \in \mathcal{E}_1 \times \mathcal{E}_2 | e_1 \equiv e_2\}$ , where  $\equiv$  refers to the equivalence relation.  $\mathcal{E}_1$  and  $\mathcal{E}_2$  are the entity sets of the respective KGs.

### 3.2 Hubness

There are several ways to measure hubness. The oldest approach (Radovanović et al., 2010) measures the skewness in the  $k$ -occurrence  $O^k$ :

$$S^k = \mathbb{E}[(O^k - \mu_{O^k})^3] / \sigma_{O^k}^3. \quad (2)$$

In this equation  $\mathbb{E}$  is the expected value,  $\mu$  indicates the mean and  $\sigma$  the standard deviation. Because this  $k$ -skewness is difficult to interpret (Feldbauer et al.,

2018) adapted an income inequality measure called *Robin Hood* index to calculate  $k$ -occurrence inequality

$$\mathcal{H}^k = \frac{1}{2} \frac{\sum_{x \in D} |O^k(x) - \mu_{O^k}|}{(\sum_{x \in D} O^k(x)) - k} = \frac{\sum_{x \in D} |O^k(x) - k|}{2k(n-1)}, \quad (3)$$

where  $D$  is a dataset of size  $n$ . The authors point out that this measure is easily interpretable, since it answers the question: "What share of 'nearest neighbor slots' must be redistributed to achieve  $k$ -occurrence equality among all objects?" (Feldbauer et al., 2018).

### 3.3 Hubness Reduction

For aligning two KGs we are interested in finding the most similar entities between the KGs. Let  $\mathbb{K}_s, \mathbb{K}_t$  be the embeddings of the two KGs we want to align. Given a distance measure  $d_{x,y}$ , where  $\mathbf{x} \in \mathbb{K}_s$  and  $\mathbf{y} \in \mathbb{K}_t$  we will refer to the  $k$  points with the lowest distance to  $x$  as it's  $k$ -nearest neighbors.

In the following we will present our open-source framework for hubness reduction for entity alignment. Our implementation relies on an adaptation of (Feldbauer et al., 2020) for our use-case. An overview of the workflow of our framework is shown in Figure 1. Given two KGEs of the data sources we wish to align, we first retrieve a number of kNN candidates using a primary distance measure (e.g. euclidean). We need kNN candidates for all  $x \in \mathbb{K}_s$ , as well as  $y \in \mathbb{K}_t$ . Bear in mind, that while the distance between such two points  $x$  and  $y$  is the same no matter whether  $x$  is a kNN candidate of  $y$  or vice versa, due to hubness  $x$  might be a kNN candidate of  $y$  but not the other way round. Using these primary distances we can apply hubness reduction methods to obtain secondary distances. These secondary distances are used to obtain the final kNN from the kNN candidates. We implemented the possibility to use approximate nearest neighbor libraries to obtain the primary distances. As we will see in Section 4, this gives a speed advantage on larger datasets. More information about the ANN approaches is given in Section 3.4.

In the following we present the hubness reduction approaches we implemented, which were the best performing techniques reported in (Feldbauer and Flexer, 2019). *Local Scaling* (LS) was first introduced in (Zelnik-Manor and Perona, 2004) and later discovered to reduce hubness (Schnitzer et al., 2012). Given a distance  $d_{x,y}$  it calculates the pairwise secondary distance

$$LS(d_{x,y}) = 1 - \exp\left(-\frac{d_{x,y}^2}{\sigma_x \sigma_y}\right) \quad (4)$$

where  $\sigma_x$  (or resp.  $\sigma_y$ ) is the distance between  $x$  (resp.  $y$ ) and their  $k$ th-nearest neighbor

Closely related to local scaling is the *non-iterative contextual dissimilarity measure* (NICDM) (Jégou et al., 2007) which was first applied to hubness reduction in the same study as LS (Schnitzer et al., 2012):

$$NICDM(d_{x,y}) = \frac{d_{x,y}}{\sqrt{\mu_x \mu_y}}, \quad (5)$$

with  $\mu_x$  being the mean distance to the  $k$ -nearest neighbors of  $x$  and analogously for  $y$  and  $\mu_y$ . *Cross-domain similarity local scaling* (CSLS) (Lample et al., 2018) was introduced to reduce hubness in word embeddings. As the previous approaches it relies on scaling locally:

$$CSLS(d_{x,y}) = 2 \cdot d_{x,y} - \mu_x - \mu_y \quad (6)$$

with  $\mu_x$  being the mean distance from  $x$  to its  $k$ -nearest neighbors. This measure was shown in (Sun et al., 2020b) to successfully reduce hubness in knowledge graph embeddings.

*Mutual Proximity* (MP) (Schnitzer et al., 2012) counts the distances of entities whose distances to both  $x$  and  $y$  are larger than  $d_{x,y}$ :

$$MP_{emp}(d_{x,y}) = \frac{|\{j : d_{x,j} > d_{x,y}\} \cap \{j : d_{y,j} > d_{y,x}\}|}{n-2} \quad (7)$$

The version in Equation 7 was adapted by (Feldbauer and Flexer, 2019) to normalize the range to  $[0, 1]$ . Since this measure is computationally expensive an approximation can be used, that relies on estimating the sample mean  $\hat{\mu}_x$  and variance  $\hat{\sigma}_x$  of the distances of all other objects to  $x$ :

$$MP_{Gauss}(d_{x,y}) = SF(d_{x,y}, \hat{\mu}_x, \hat{\sigma}_x^2) \cdot SF(d_{x,y}, \hat{\mu}_y, \hat{\sigma}_y^2). \quad (8)$$

In this equation  $SF$  is the complement to the cumulative density function at  $d_{x,y}$ .

The final hubness reduction method we implemented is *DSL* (Hara et al., 2016). This technique relies on flattening the density gradient, by estimating the local centroids  $c_k(x) = \frac{1}{k} \sum_{x' \in kNN(x)} x'$ , with  $kNN(x)$  being the set of  $k$ -nearest neighbors of  $x$ . This leads to the following formula:

$$DSL(x,y) = \|x-y\|_2^2 - \|x-c_k(x)\|_2^2 - \|x-c_k(y)\|_2^2. \quad (9)$$

### 3.4 Approximate Nearest Neighbors

Due to the relatively high time complexity of hubness reduction methods and the successful use of approximate nearest neighbor (ANN) approaches to mitigate this problem (Feldbauer et al., 2018), we utilize three ANN algorithms for our study:

- *HNSW* (Malkov, 2018) is an extension of navigable small world graphs, that exploits a hierarchical structure of proximity graphs.

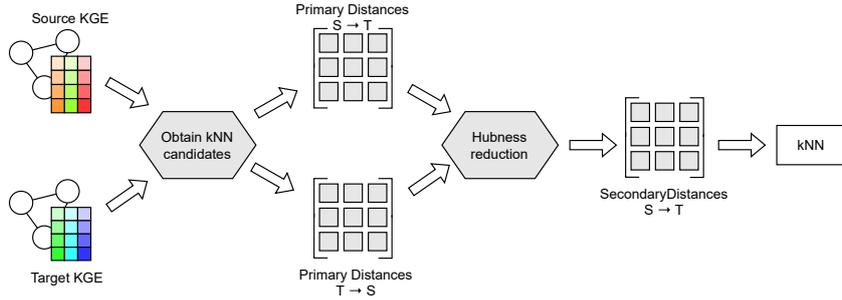


Figure 1: Overview of our framework.

- *NGT* (Iwasaki, 2016) relies on the kNN graph for indexing and greedy search.
- *Annoy*<sup>1</sup> is a tree-based approach, which splits the dataset subsequently into smaller sections for each node.

For a general benchmark of ANN algorithms see (Aumüller et al., 2020).

## 4 EVALUATION

The evaluation section begins with an overview of our experimental setup including the datasets and embedding approaches as well as configurations. Afterwards, we present our results in detail.

### 4.1 Evaluation Setup

The 16 alignment tasks we use for evaluation were presented in (Sun et al., 2020b) and consist of samples from DBpedia (D), Wikidata (W) and Yago (Y). These fragments of KGs contain a wide range of different relationships and entity types, as well as covering cross-lingual settings (EN-DE & EN-FR). There are two sizes of datasets, depending on the number of entities: 15K and 100K. More information about the datasets is shown in Table 1. The number of entities in the respective datasets is equal to the size of the respective  $\mathcal{M}$ , which means the task consists of finding a 1-1 alignment of entities between the two datasets. Be aware, that we use an updated version of the datasets<sup>2</sup>, which explains different results between our evaluation and the findings of (Sun et al., 2020b). We however used the same hyperparameter settings to create the KGEs as said study.

To create the KGEs of these datasets we used a wide range of embedding approaches implemented in

<sup>1</sup><https://github.com/spotify/annoy>

<sup>2</sup><https://github.com/nju-websoft/OpenEA#dataset-overview>

Table 1: Statistics of datasets.

			15K			100K		
			$\mathcal{T}$	$\mathcal{P}$	$\mathcal{L}$	$\mathcal{T}$	$\mathcal{P}$	$\mathcal{L}$
D-W	V1	D	90399	589	28237	628901	905	133931
		W	180992	818	118515	939568	1135	542921
	V2	D	125361	341	25690	977153	645	137483
		W	259051	578	146977	1466422	999	682367
D-Y	V1	D	82384	421	25297	654603	665	101386
		Y	143752	62	105710	1050305	69	497633
	V2	D	117665	161	22561	951332	506	97433
		Y	177121	40	104546	1620426	66	578596
EN-DE	V1	DE	184195	324	35630	922447	447	199527
		EN	110079	500	28973	759025	831	147142
	V2	DE	253947	211	33185	1285853	358	200356
		EN	144378	339	23831	1053340	648	139867
EN-FR	V1	EN	104498	574	30281	693855	865	145103
		FR	95265	613	28760	599010	818	157791
	V2	EN	148714	381	22761	1046052	742	145382
		FR	136226	386	21645	904159	754	157564

Table 2: Embedding approaches used in the evaluation.

Approach	Method	Lit.
AttrE (Trisedya et al., 2019)	Translation	yes
BootEA (Sun et al., 2018)	Translation	-
ConvE (Dettmers et al., 2018)	Neural	-
GCNAlign (Wang et al., 2018)	Neural	yes
HolE (Nickel et al., 2016)	Factorization	-
IMUSE (He et al., 2019)	Translation	yes
IPTransE (Zhu et al., 2017)	Path	-
JAPE (Sun et al., 2017)	Translation	yes
MultiKE (Zhang et al., 2019)	Translation	yes
ProjE (Shi and Weninger, 2017)	Neural	-
RSN4EA (Guo et al., 2019)	Path	-
RotatE (Sun et al., 2019)	Factorization	-
SimplE (Kazemi and Poole, 2018)	Factorization	-
TransD (Ji et al., 2015)	Translation	-
TransH (Wang et al., 2014)	Translation	-

the framework OpenEA<sup>3</sup>. Table 2 shows a summary of the 15 embedding approaches. With the 16 alignment tasks and 15 embedding approaches we therefore have 240 KGE pairs for our study.

For the exact nearest neighbor search we used the scikit-learn (Pedregosa et al., 2011) implementations of *Ball Tree* (Omohundro, 1989), *KD-Tree* (Bentley, 1975) and their *brute-force* variant which does not exploit metric space advantages. The approxi-

<sup>3</sup><https://github.com/nju-websoft/OpenEA>

mate nearest neighbor algorithms used were Annoy, NGT and HNSW. For all algorithms we found, that their default settings gave the best results, except for HNSW where the hyperparameters  $M = 96$  and  $efConstruction = 500$  showed the best results. More details can be found in our benchmarking repository <https://github.com/dobraczka/kiez-benchmarking>.

Our experiment setting consists of doing a full alignment between the data sources, i.e. finding the  $k$  nearest neighbors of all the source entities in the target entity embeddings. We choose  $k = 50$  and allowed 100 kNN candidates to obtain the primary distances. The primary distance was euclidean for all algorithms, except for HNSW, where it was cosine.

For all experiments we used a single machine running CentOS 7 with 4 AMD EPYC 7551P 32-Core CPUs. For the small dataset experiments we allowed 10GB of RAM. The experiments with the large datasets were provided 30GB of RAM.

To evaluate the retrieval quality of the different techniques we use the  $hits@k$  metric:

$$hits@k(kNN) = \frac{|\{t : y \in kNN(x) \wedge (x, y) \in \mathcal{M}\}|}{|\mathcal{M}|}, \quad (10)$$

where  $kNN$  are the calculated nearest neighbors and  $kNN(x)$  returns the  $k$  nearest neighbors of  $x$ . This metric simply counts the proportion of true matches  $t$  in the  $k$  nearest neighbors. While precision and recall are the most common metrics for data integration tasks we choose  $hits@k$ , because it is the common metric for entity alignment tasks and is a better measure of quality for neighbor-based tasks. In our case we present  $hits@50$ , since we wanted the 50 nearest neighbors.

Our evaluation is driven by three major questions:

- (Q<sub>1</sub>): Does hubness reduction improve the alignment accuracy?
- (Q<sub>2</sub>): Does hubness reduction offset loss in retrieval quality by ANN algorithms?
- (Q<sub>3</sub>): Can hubness reduction be used with ANN algorithms without loss of the speed advantage of ANNs?

## 4.2 Results

### 4.2.1 Hubness Reduction with Exact Nearest Neighbors

The initial quality of the KGEs plays a major role in the absolute  $hits@k$  value. To address (Q<sub>1</sub>) we will therefore look at the  $hits@k$  improvement of hubness reduction methods compared to the baseline of using

no hubness reduction. We present a boxplot representation of the results in Figure 2, which summarizes the results over all embedding approaches per alignment task. It is evident, that all hubness reduction methods tend to improve the results. There are however differences between the approaches. We can see for example that the two Mutual Proximity variants perform the worst. In order to make statistically sound statements about differences between approaches we rely on the statistical analysis presented by Demšar (Demšar, 2006) and the Python package Autorank (Herbold, 2020), which makes these best practices readily available. Since we have more than two hubness reduction methods this means we first test if the average ranks of the methods are significantly different using the Friedman test. We do this for the results across all datasets and embedding approaches. If we can determine significant differences in the results we perform a post-hoc Nemenyi test to make a pairwise comparison of hubness reduction methods. The resulting critical distance diagram is shown in Figure 3. The lower the rank of the approach the better. Connected groups are not significantly different at significance level  $\alpha = 0.05$ . With exception of DSL and CSLS all approaches perform significantly different from another. We can especially see that NICDM is significantly better than all other approaches. Our (Q<sub>1</sub>) is therefore answered.

Given the large variance seen in Figure 2 the improvements are very different between embedding approaches. We therefore take a closer look at some selected approaches in Figure 4. First of all we can see that there is a large difference in the hubness produced by the three selected embedding approaches. While BootEA has relatively low hubness even without hubness reduction, Simple has a Robin Hood index of almost 75% percent. This means that for the latter almost 75% of nearest neighbor slots would have to be redistributed to obtain  $k$ -occurrence equality. Since BootEA’s  $hits@50$  score is already very high there is little room for improvement through hubness reduction. However for the two other approaches we can see that hubness reduction can improve the  $hits@50$  noticeably.

### 4.2.2 Hubness Reduction with Approximate Nearest Neighbors

To answer (Q<sub>2</sub>) we compare the improvement of  $hits@50$  relative to the baseline with the same baseline as before (exact NN search without hubness reduction). Figure 5 again summarizes these results over all embedding approaches as boxplot. In contrast to Figure 2 we can see that there are many cases, where the results are worse than the baseline, i.e. neg-

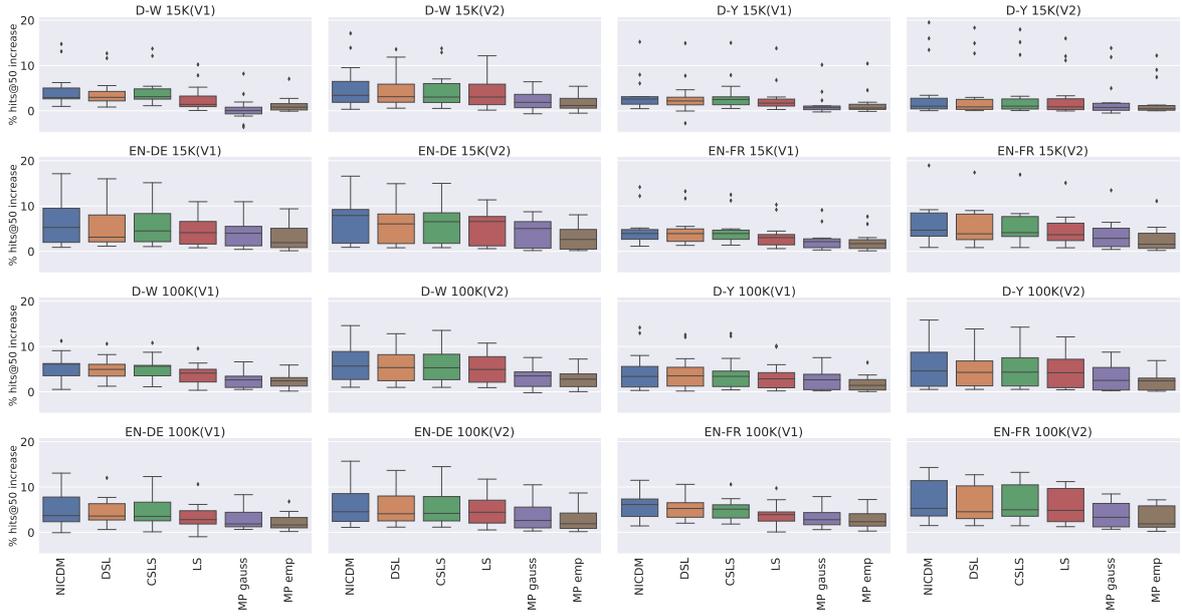


Figure 2: Improvement in hits@50 compared to no hubness reduction. Results are aggregated over different embedding approaches.

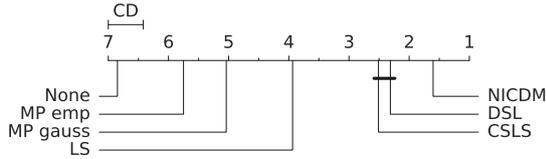


Figure 3: Critical distance diagram for different hubness reduction techniques w.r.t hits@50. Approaches that are not significantly different at  $\alpha = 0.05$  are connected. Low ranks are better.

ative improvement. Especially Annoy tends to perform worse than the baseline and it has the highest variance of all three approaches. HNSW seems to perform the best with almost all results staying in the positive range. To make more substantial statements we will again use our aforementioned statistical testing procedure. To make the critical distance diagram less cluttered we only compare the the three best hubness reduction methods from Figure 3 with the baseline. The resulting critical distance diagram is shown in Figure 6. There is no significant difference between Annoy and the baseline. NGT with DSL and CSLS is also not significantly different from the baseline. HNSW with DSL and NICDM performs the best and is significantly different from all other approaches. The answer to (Q<sub>2</sub>) is therefore nuanced: While not all ANN algorithms can achieve the same quality as the baseline, given the right algorithm and hubness reduction technique we can not only match the performance of exact NN algorithms, but we can significantly outperform them.

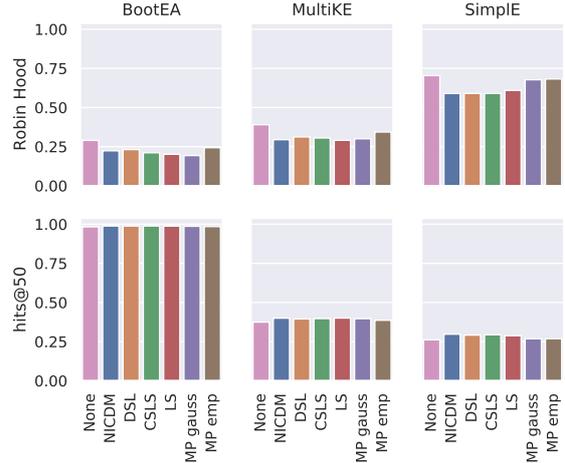


Figure 4: Robin Hood index and hits@50 for selected embedding approaches on D-Y 100K(V2) dataset.

### 4.2.3 Execution Time

To answer our last research question we investigate the difference in execution time for the large and small datasets separately. The results are shown in Figure 7. Generally we can see that Annoy is the fastest approach, however, as mentioned before, the low accuracy in terms of hits@50 disqualifies it for our use case. Surprisingly, the brute approach is the fastest *exact* algorithm on all our datasets. On the small datasets Brute is the fastest high-quality approach without hubness reduction and has similar ex-

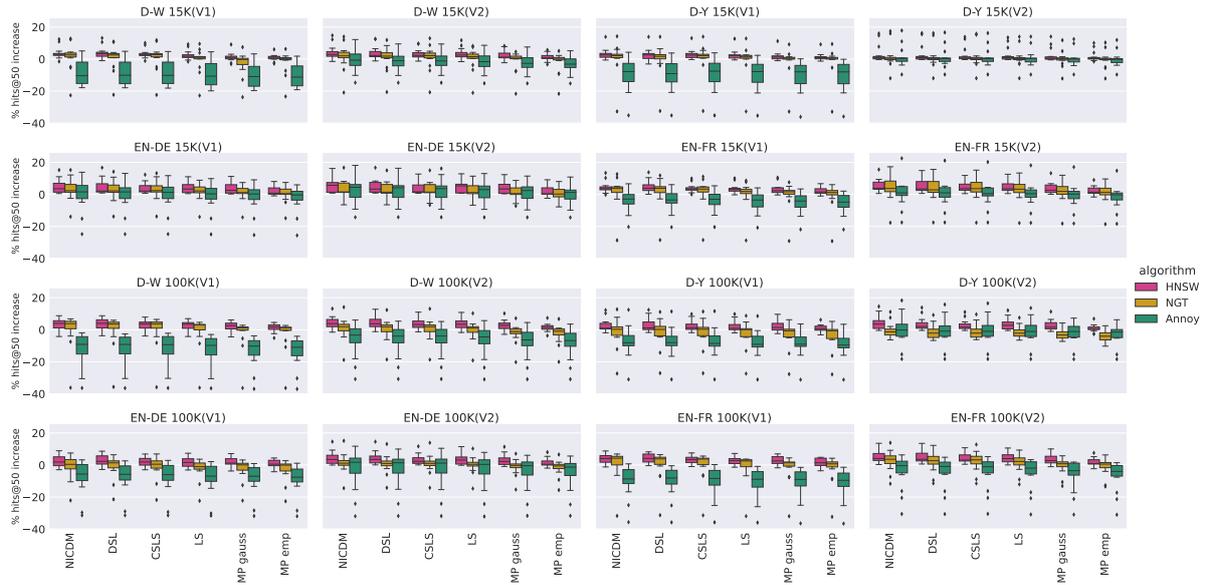


Figure 5: Improvement in hits@50 compared to using no hubness reduction with an exact NN algorithm. Results are aggregated over different embedding approaches.

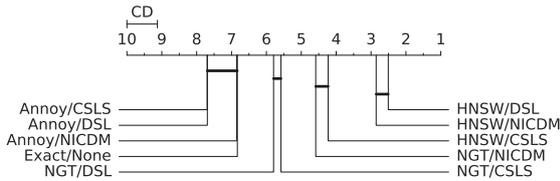


Figure 6: Critical distance diagram for different algorithms and hubness reduction techniques with regards to hits@50. Approaches that are not significantly different at  $\alpha = 0.05$  are connected. Low ranks are better.

execution time as HNSW, when hubness reduction is used. Looking at the 100K datasets, we see the clear speed advantage of the ANN algorithms. For our significance test we are interested to determine speed advantages of high-quality algorithm/hubness reduction combinations. We therefore ignore Annoy in the critical distance diagram shown in Figure 8. We can see that except for NGT with DSL all approaches are significantly faster than the baseline (Exact/None). HNSW with NICDM is significantly faster than all other approaches except HNSW with CSLS.

#### 4.2.4 Additional Results

Given our results for the 50 nearest neighbors we are also able to determine hits@k scores for different  $k$  values. In Figure 9 we show results for hits@{1,10,25}. For space reasons we show boxplots, that aggregate the results over all datasets and embedding approaches. For a more granular presenta-

tion we refer to a report in our benchmark repository<sup>4</sup>.

We can see in the boxplots, that the quality increase tends to be higher the lower  $k$  gets. For example the median increase of HNSW with the hubness reduction method NICDM is:

- 5.5% w.r.t hits@25
- 8.43% w.r.t hits@10
- 12.41% w.r.t hits@1

This makes sense because entities that are hubs tend to occupy the most important nearest neighbor slots. The increased variance with lower  $k$  is due to the fact, that hits@k values tend get lower the lower  $k$  gets, because it is a more difficult task. This leaves more room for possible improvement.

The biggest change we can see between different  $k$  values is the performance of the DSL hubness reduction technique. We suppose that the reason for this is that we ran our experiments for  $k=50$  and set DSL's  $k$  parameter accordingly (see Eq. 9).

Another important observation is the improved performance of Annoy w.r.t hits@1 in contrast to hits@50. While Annoy still has a higher variance than HNSW it's results are comparable, but as stated before Annoy is much faster. Our general recommendations are therefore to use NICDM as hubness reduction technique and depending on the desired number of kNN either HNSW for  $k > 1$  or Annoy for  $k = 1$ .

<sup>4</sup>[https://github.com/dobraczka/kiez-benchmarking/blob/main/results/additional\\_report.pdf](https://github.com/dobraczka/kiez-benchmarking/blob/main/results/additional_report.pdf)

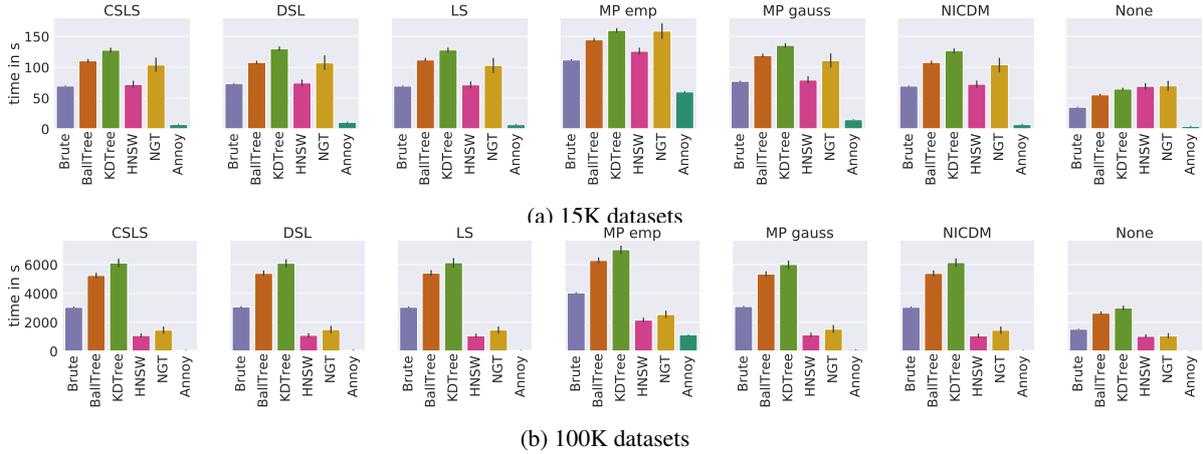


Figure 7: Time in seconds for different (A)NN algorithms and hubness reduction methods. Results are averaged over datasets with black bar showing variance.

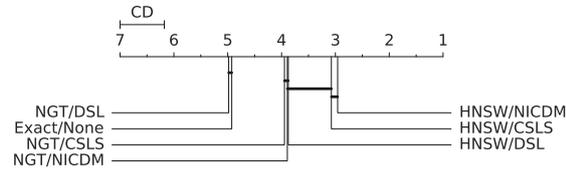


Figure 8: Critical distance diagram for different algorithms and hubness reduction techniques with regards to execution time. Approaches that are not significantly different at  $\alpha = 0.05$  are connected. Low ranks are better.

## 5 CONCLUSION & FUTURE WORK

In this study we investigated the advantages of using hubness reduction techniques for entity alignment with knowledge graph embeddings. Our results suggest that using methods to mitigate hubness improves alignment results significantly. This is also true when comparing ANN algorithms to the baseline of using no hubness reduction and exact NN algorithms. Using the ANN algorithm HNSW together with the hubness reduction technique NICDM gives a median improvement in hits@50 of 3.18% and for large datasets a median speedup of 1.88x. For small datasets the execution time of HNSW with NICDM is similar to the brute-force variant with NICDM.

We noticed even higher improvements in hits@1, e.g. for HNSW with NICDM a median improvement of 12.41% compared to the baseline. Given the high improvements in terms of hits@1 it could be beneficial to utilize the hubness reduced distances as input for clustering-based matchers (Saeedi et al., 2017).

Since KGEs are usually generated with the help of known entity matches a worthwhile future investi-

gation could be the utilization of this training data in the hubness reduction as well as to calculate the nearest neighbors. Because KGEs are commonly trained with the aid of GPUs investigating ANN libraries that make use of this available resource could further increase the speed advantage of ANN algorithms on the task of entity alignment with KGEs.

## ACKNOWLEDGEMENTS

This work was supported by the German Federal Ministry of Education and Research (BMBF, 01/S18026A-F) by funding the competence center for Big Data and AI "ScaDS.AI Dresden/Leipzig". Some computations have been done with resources of Leipzig University Computing Center.

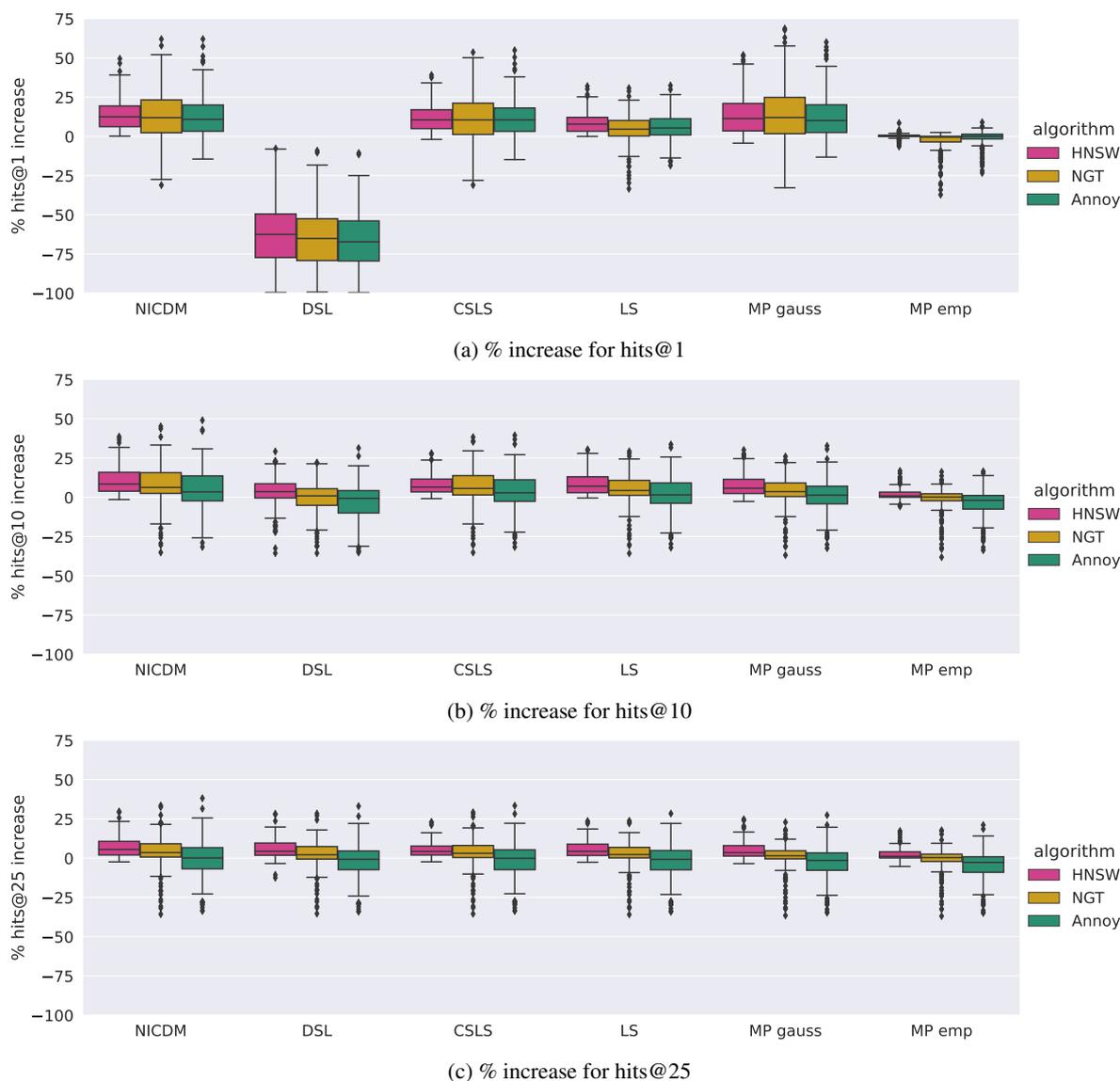


Figure 9: Increase in hits@{1,10,25} compared to baseline (exact NN algorithm without hubness reduction). Boxplot presentation shows aggregated results over different embedding approaches and all datasets.

## REFERENCES

- Aggarwal, C. C., Hinneburg, A., and Keim, D. A. (2001). On the surprising behavior of distance metrics in high dimensional space. *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, 1973:420–434.
- Ali, M., Berrendorf, M., Hoyt, C. T., Vermue, L., Galkin, M., Sharifzadeh, S., Fischer, A., Tresp, V., and Lehmann, J. (2020). Bringing light into the dark: A large-scale evaluation of knowledge graph embedding models under a unified framework. *CoRR*, abs/2006.13365.
- Aumüller, M., Bernhardsson, E., and Faithfull, A. (2020). ANN-Benchmarks: A benchmarking tool for approximate nearest neighbor algorithms. *Information Systems*, 87.
- Bentley, J. L. (1975). Multidimensional binary search trees used for associative searching. *Commun. ACM*, 18(9):509–517.
- Bhattacharya, I. and Getoor, L. (2007). Collective entity resolution in relational data. *ACM Trans. Knowl. Discov. Data*, 1(1):5.
- Bordes, A., Usunier, N., García-Durán, A., Weston, J., and Yakhnenko, O. (2013). Translating embeddings for modeling multi-relational data. In *Advances in Neu-*

- ral Information Processing Systems 26: 27th Annual Conference on Neural Information Processing Systems 2013. Proceedings of a meeting held December 5-8, 2013, Lake Tahoe, Nevada, United States*, pages 2787–2795.
- Christen, P. (2012). *Data Matching - Concepts and Techniques for Record Linkage, Entity Resolution, and Duplicate Detection*. Data-Centric Systems and Applications. Springer.
- Dai, Y., Wang, S., Xiong, N. N., and Guo, W. (2020). A survey on knowledge graph embedding: Approaches, applications and benchmarks. *Electronics (Switzerland)*, 9(5):1–29.
- Demšar, J. (2006). Statistical comparisons of classifiers over multiple data sets. *Journal of Machine Learning Research*, 7:1–30.
- Dettmers, T., Minervini, P., Stenetorp, P., and Riedel, S. (2018). Convolutional 2d knowledge graph embeddings. In *Proc. of AAAI*, pages 1811–1818. AAAI Press.
- Feldbauer, R. and Flexer, A. (2019). A comprehensive empirical comparison of hubness reduction in high-dimensional spaces. *Knowledge and Information Systems*, 59(1):137–166.
- Feldbauer, R., Leodolter, M., Plant, C., and Flexer, A. (2018). Fast approximate hubness reduction for large high-dimensional data. *Proceedings - 9th IEEE International Conference on Big Knowledge, ICBK 2018*, pages 358–367.
- Feldbauer, R., Rattei, T., and Flexer, A. (2020). scikit-hubness: Hubness reduction and approximate neighbor search. *Journal of Open Source Software*, 5(45):1957.
- Guo, L., Sun, Z., and Hu, W. (2019). Learning to exploit long-term relational dependencies in knowledge graphs. In *Proceedings of the 36th International Conference on Machine Learning, ICML 2019, 9-15 June 2019, Long Beach, California, USA*, volume 97 of *Proceedings of Machine Learning Research*, pages 2505–2514. PMLR.
- Hara, K., Suzuki, I., Kobayashi, K., and Fukumizu, K. (2015a). Reducing hubness: A cause of vulnerability in recommender systems. In *Proc. of SIGIR*, pages 815–818. ACM.
- Hara, K., Suzuki, I., Kobayashi, K., Fukumizu, K., and Radovanovic, M. (2016). Flattening the density gradient for eliminating spatial centrality to reduce hubness. In *Proc. of AAAI*, pages 1659–1665. AAAI Press.
- Hara, K., Suzuki, I., Shimbo, M., Kobayashi, K., Fukumizu, K., and Radovanovic, M. (2015b). Localized centering: Reducing hubness in large-sample data. In *Proc. of AAAI*, pages 2645–2651. AAAI Press.
- He, F., Li, Z., Qiang, Y., Liu, A., Liu, G., Zhao, P., Zhao, L., Zhang, M., and Chen, Z. (2019). Unsupervised entity alignment using attribute triples and relation triples. In *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, volume 11446 LNCS, pages 367–382.
- Herbold, S. (2020). Autorank: A python package for automated ranking of classifiers. *Journal of Open Source Software*, 5(48):2173.
- Huang, J., Hu, W., Bao, Z., and Qu, Y. (2020). Crowdsourced collective entity resolution with relational match propagation. In *Proc. of ICDE*, pages 37–48. IEEE.
- Iwasaki, M. (2016). Pruned Bi-directed K-nearest neighbor graph for proximity search. In *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, volume 9939 LNCS, pages 20–33.
- Jégou, H., Harzallah, H., and Schmid, C. (2007). A contextual dissimilarity measure for accurate and efficient image search. In *2007 IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR 2007), 18-23 June 2007, Minneapolis, Minnesota, USA*. IEEE Computer Society.
- Ji, G., He, S., Xu, L., Liu, K., and Zhao, J. (2015). Knowledge graph embedding via dynamic mapping matrix. In *Proc. of ACL*, pages 687–696, Beijing, China. Association for Computational Linguistics.
- Kazemi, S. M. and Poole, D. (2018). Simple embedding for link prediction in knowledge graphs. In *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada*, pages 4289–4300.
- Lample, G., Conneau, A., Ranzato, M., Denoyer, L., and Jégou, H. (2018). Word translation without parallel data. In *Proc. of ICLR*. OpenReview.net.
- Lin, Y., Liu, Z., Sun, M., Liu, Y., and Zhu, X. (2015). Learning entity and relation embeddings for knowledge graph completion. In *Proc. of AAAI*, pages 2181–2187. AAAI Press.
- Low, T., Borgelt, C., Stober, S., and Nürnberger, A. (2013). The hubness phenomenon: Fact or artifact? *Studies in Fuzziness and Soft Computing*, 285:267–278.
- Malkov, Y. A. (2018). Efficient and robust approximate nearest neighbor search using Hierarchical Navigable Small World graphs. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, pages 31–33.
- Nickel, M., Rosasco, L., and Poggio, T. A. (2016). Holographic embeddings of knowledge graphs. In *Proc. of AAAI*, pages 1955–1961. AAAI Press.
- Nickel, M., Tresp, V., and Kriegel, H. (2011). A three-way model for collective learning on multi-relational data. In *Proceedings of the 28th International Conference on Machine Learning, ICML 2011, Bellevue, Washington, USA, June 28 - July 2, 2011*, pages 809–816. Omnipress.
- Omohundro, S. M. (1989). Five balltree construction algorithms. Technical report, International Computer Science Institute.
- Pachet, F. and Aucouturier, J.-J. (2004). Improving timbre similarity: How high is the sky. *Journal of negative results in speech and audio sciences*, 1(1).
- 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.
- Pershina, M., Yakout, M., and Chakrabarti, K. (2015). Holistic entity matching across knowledge graphs. In *2015 IEEE International Conference on Big Data, Big Data 2015, Santa Clara, CA, USA, October 29 - November 1, 2015*, pages 1585–1590. IEEE Computer Society.
- Radovanovic, M., Nanopoulos, A., and Ivanovic, M. (2009). Nearest neighbors in high-dimensional data: the emergence and influence of hubs. In *Proceedings of the 26th Annual International Conference on Machine Learning, ICML 2009, Montreal, Quebec, Canada, June 14-18, 2009*, volume 382 of *ACM International Conference Proceeding Series*, pages 865–872. ACM.
- Radovanović, M., Nanopoulos, A., and Ivanović, M. (2010). Hubs in space: Popular nearest neighbors in high-dimensional data. *Journal of Machine Learning Research*, 11.
- Saeedi, A., Peukert, E., and Rahm, E. (2017). Comparative evaluation of distributed clustering schemes for multi-source entity resolution. In *Advances in Databases and Information Systems - 21st European Conference, ADBIS 2017, Nicosia, Cyprus, September 24-27, 2017, Proceedings*, volume 10509 of *Lecture Notes in Computer Science*, pages 278–293. Springer.
- Schnitzer, D., Flexer, A., Schedl, M., and Widmer, G. (2012). Local and global scaling reduce hubs in space. *Journal of Machine Learning Research*, 13.
- Shi, B. and Weninger, T. (2017). Proje: Embedding projection for knowledge graph completion. In *Proc. of AAAI*, pages 1236–1242. AAAI Press.
- Sun, R., Cao, X., Zhao, Y., Wan, J., Zhou, K., Zhang, F., Wang, Z., and Zheng, K. (2020a). Multi-modal knowledge graphs for recommender systems. In *CIKM '20: The 29th ACM International Conference on Information and Knowledge Management, Virtual Event, Ireland, October 19-23, 2020*, pages 1405–1414. ACM.
- Sun, Z., Deng, Z., Nie, J., and Tang, J. (2019). Rotate: Knowledge graph embedding by relational rotation in complex space. In *Proc. of ICLR*. OpenReview.net.
- Sun, Z., Hu, W., and Li, C. (2017). Cross-lingual entity alignment via joint attribute-preserving embedding. *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, 10587 LNCS:628–644.
- Sun, Z., Hu, W., Zhang, Q., and Qu, Y. (2018). Bootstrapping entity alignment with knowledge graph embedding. In *Proceedings of the Twenty-Seventh International Joint Conference on Artificial Intelligence, IJCAI 2018, July 13-19, 2018, Stockholm, Sweden*, pages 4396–4402. ijcai.org.
- Sun, Z., Zhang, Q., Hu, W., Wang, C., Chen, M., Akrami, F., and Li, C. (2020b). A benchmarking study of embedding-based entity alignment for knowledge graphs. *Proc. VLDB Endow.*, 13(11):2326–2340.
- Suzuki, I., Hara, K., Shimbo, M., Saerens, M., and Fukumizu, K. (2013). Centering similarity measures to reduce hubs. In *Proc. of EMNLP*, pages 613–623, Seattle, Washington, USA. Association for Computational Linguistics.
- Tomašev, N. and Buza, K. (2015). Hubness-aware knn classification of high-dimensional data in presence of label noise. *Neurocomputing*, 160:157–172.
- Trisedya, B. D., Qi, J., and Zhang, R. (2019). Entity Alignment between Knowledge Graphs Using Attribute Embeddings. *Proc. of AAAI*, 33:297–304.
- Usbeck, R., Röder, M., Hoffmann, M., Conrads, F., Huthmann, J., Ngomo, A. N., Demmler, C., and Unger, C. (2019). Benchmarking question answering systems. *Semantic Web*, 10(2):293–304.
- Vincent, E., Gkiokas, A., Schnitzer, D., and Flexer, A. (2014). An investigation of likelihood normalization for robust ASR. In *INTERSPEECH 2014, 15th Annual Conference of the International Speech Communication Association, Singapore, September 14-18, 2014*, pages 621–625. ISCA.
- Wang, Z., Lv, Q., Lan, X., and Zhang, Y. (2018). Cross-lingual knowledge graph alignment via graph convolutional networks. In *Proc. of EMNLP*, pages 349–357, Brussels, Belgium. Association for Computational Linguistics.
- Wang, Z., Zhang, J., Feng, J., and Chen, Z. (2014). Knowledge graph embedding by translating on hyperplanes. In *Proc. of AAAI*, pages 1112–1119. AAAI Press.
- Zelnik-Manor, L. and Perona, P. (2004). Self-tuning spectral clustering. In *Advances in Neural Information Processing Systems 17 [Neural Information Processing Systems, NIPS 2004, December 13-18, 2004, Vancouver, British Columbia, Canada]*, pages 1601–1608.
- Zhang, Q., Sun, Z., Hu, W., Chen, M., Guo, L., and Qu, Y. (2019). Multi-view knowledge graph embedding for entity alignment. In *Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI 2019, Macao, China, August 10-16, 2019*, pages 5429–5435. ijcai.org.
- Zhu, H., Xie, R., Liu, Z., and Sun, M. (2017). Iterative entity alignment via joint knowledge embeddings. In *Proceedings of the Twenty-Sixth International Joint Conference on Artificial Intelligence, IJCAI 2017, Melbourne, Australia, August 19-25, 2017*, pages 4258–4264. ijcai.org.