

Application of Concepts of Neighbours to Knowledge Graph Completion¹

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Abstract. The open nature of Knowledge Graphs (KG) often implies that they are incomplete. Knowledge graph completion (aka. link prediction) consists in inferring new relationships between the entities of a KG based on existing relationships. Most existing approaches rely on the learning of latent feature vectors for the encoding of entities and relations. In general however, latent features cannot be easily interpreted. Rule-based approaches offer interpretability but a distinct ruleset must be learned for each relation. In both latent- and rule-based approaches, the training phase has to be run again when the KG is updated. We propose a new approach that does not need a training phase, and that can provide interpretable explanations for each inference. It relies on the computation of Concepts of Nearest Neighbours (C-NN) to identify clusters of similar entities based on common graph patterns. Different rules are then derived from those graph patterns, and combined to predict new relationships. We evaluate our approach on standard benchmarks for link prediction, where it gets competitive performance compared to existing approaches.

Keywords: Knowledge Graph, Multi-Relational Data, Knowledge Graph Completion, Link Prediction, Graph Pattern, Concepts of Nearest Neighbours, Inference Rules, Analogical Inference, Explainable AI

1. Introduction

There is a growing interest for knowledge graphs (KG) as a way to represent and share data on the Web. The Semantic Web [2] defines standards for representation (RDF), querying (SPARQL), and reasoning (RDFS, OWL), and thousands of open KGs are available: e.g., DBpedia, Wikidata (formerly Freebase), YAGO, WordNet. The open nature of KGs often implies that they are incomplete, and a lot of work have studied the use of machine learning techniques to complete them.

The task of *knowledge graph completion*, aka. *link prediction* [3], consists in predicting missing edges or missing parts of edges. It is therefore a form of machine learning. Suppose that film *Avatar* is missing a director in the KG, one wants to predict it, i.e. identify it among all KG nodes. The idea is to find regularities in the existing knowledge, and to exploit them in order to rank KG nodes. The higher the correct node is in the ranking, the better the prediction is. Link prediction was originally introduced for social networks with a single edge type (a single *relation*) [4], and was later extended to multi-relational data and applied to KGs [3]. Compared to the classical task of supervised classification, knowledge graph completion faces several challenges. First, there are as many classification problems as there are relations, which count in the hundreds or thousands in KGs. Second, for each relation, the number of “classes” is the number of different *entities* in the range of the relation, which typically counts in the

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1 thousands for relations like *spouse* or *birthPlace*. Third, some relations can be multi-valued, like the
2 relation from films to actors.

3 In this paper, we report on extensive experimental results about a novel approach to knowledge graph
4 completion that is based on *Concepts of Nearest Neighbours (C-NN)*, which were introduced in [5], and
5 applied to *query relaxation* in [6]. This paper is an extended version of [1] that reports on first results
6 about the application of C-NNs to link prediction. In particular, the extension includes an analogical
7 form of inference, and an extensive and deeper experimental evaluation. The C-NN approach introduces
8 a symbolic form of k-NN (k Nearest Neighbours) where numerical distances are replaced by graph
9 patterns that provide an intelligible representation of how similar two entities are.

10 Our hypothesis is that the partitioning of the KG entities into concepts of neighbours (see Section 5)
11 provides a valuable basis for different kinds of inferences. We here focus on knowledge graph comple-
12 tion, i.e. the inference of the missing node of an incomplete edge.

13 The contribution of this work is a novel approach to knowledge graph completion that has the follow-
14 ing properties:

- 15 (1) it is a form of *instance-based learning*, i.e. it can perform inferences without training, and hence
16 accomodate new data without re-training;
- 17 (2) it is a *symbolic approach*, i.e. it can provide explanations for each inference;
- 18 (3) it shows *competitive performance* on standard link prediction benchmarks.

19
20 The rest of the paper is organized as follows. Section 2 discusses related work on knowledge graph
21 completion. Section 3 contains preliminaries about knowledge graphs and queries. Section 4 presents
22 an overview of our approach. Section 5 recalls the definition of C-NNs, and their efficient computation.
23 Section 6 presents our method to perform C-NN-based knowledge graph completion. Section 7 reports
24 on positive experimental results on standard benchmarks (WN18, WN18RR, FB15k, FB15k-237), along
25 with an in-depth analysis of results. Finally, Section 8 concludes and sketches future work.

27 28 2. Related Work

29
30 Nickel *et al* [3] published a “review of relational machine learning for knowledge graphs”, where link
31 prediction is the main inference task. They identify two kinds of approaches that differ by the kind of
32 model they use: *latent feature models*, and *graph feature models*. The former is by far the most studied
33 one. Before going into details, it is useful to set the vocabulary as it is used in the domain. Nodes are
34 called *entities*, edge labels are called *relations*, and edges are called *triples* (e_i, r_k, e_j) , where e_i is the
35 *head* entity, e_j is the *tail* entity, and r_k is the relation that links the head to the tail.

36 Latent feature models learn *embeddings* of entities and relations into low-dimensional vector spaces,
37 and then make inferences about a triple (e_i, r_k, e_j) by combining the embeddings of the two entities and
38 the embedding of the relation. The existing methods vary by how they learn the embeddings, and how
39 they combine them. Those methods are based on a range of techniques including: matrix factoriza-
40 tion, tensor factorization, neural networks, and gradient descent. For example, one of the first method
41 for KGs, TransE [7], models a relation as a translation in the embedding space of entities, and scores
42 a candidate triple according to the distance between the translated head and the tail. The authors of
43 TransE, Bordes *et al*, introduced two datasets, FB15k and WN18, respectively derived from Freebase
44 and WordNet, which became benchmarks in the evaluation of link prediction methods. Toutanova and
45 Chen [8] however showed that a very simple method was able to outperform previous methods because
46

of a flaw in the datasets: many test triples have their inverse among the training triples. They introduced a challenging subset of FB15k, called FB15k-237, where all inverse triples are removed. Dettmers [9] introduced a similar subset of WN18, called WN18RR. Lately, performance was significantly improved on the challenging FB15k-237 by using convolutional architectures to learn embeddings [10] or to combine the embeddings in scoring functions [9]. The state-of-the-art results are obtained by ComplEx-N3, combining low-rank tensor decomposition with the addition of inverse relations, and various optimizations about hyper-parameters and regularization [11]. The task of link prediction has also been extended with the embedding model RAE to *multi-fold relations* (aka. n-ary relations), and to *instance reconstruction* where only one entity of an n-ary relation is known, and all other entities have to be inferred together [12]. In this work, we limit ourselves to binary relations, and let those advanced cases to future work.

The latent feature models face two major drawbacks for their application to real settings. First, as they rely on the learning of entity embeddings, they cannot be applied to unseen entities, and the model has to be retrained whenever new entities or relations are introduced in the knowledge graph. Second, the predictions come without any explanation, and the meaning of learned latent features generally remain obscure. Given that it is unrealistic to expect high precision knowledge graph completion, simply because some of the missing information cannot be inferred from existing knowledge, human curation is necessary in practice. An explanation can comfort the curator in the veracity of the prediction, and could even be used to define automated inference rules.

Graph feature models, also called *observed feature models*, make inferences directly from the observed edges in the KG. Random walk inference [13] takes relation paths as features, and sets the feature values through random walks in the KG. The feature weights are learned by logistic regression for each target relation, and then used to score the candidate triples. The method has shown improvement over Horn clause generation with ILP (Inductive Logic Programming) [14]. AMIE+ [15] manages to generate such Horn clauses in a much more efficient way by designing new ILP algorithms tailored to KGs. They also introduce a novel rule measure that improves the inference precision under the Open World Assumption (OWA) that holds in KGs. A fine-grained evaluation [16] has shown that rule-based approaches are competitive with latent-based approaches, both in performance and in running time. AnyBURL [17] restricts to path-like Horn clauses, and employs an anytime bottom-up strategy for learning rules. It significantly improves performance compared to AMIE+, and gets close to the state-of-the-art of latent feature models. Graph feature models, especially rule-based approaches, offer the advantage to produce intelligible explanations for inferences, unlike the latent feature models. Moreover, they can be applied to unseen entities because inferences are based on the neighborhood of the entity in the knowledge graph, rather than on a learned embedding. However, they require a distinct training phase for each of the possibly many target relations, whereas the latent feature models are generally learned in one training phase. A drawback of both kinds of approaches is that new embeddings and new rulesets need to be learned whenever the KG is updated, which becomes a challenge for dynamic data.

Our approach relies on graph features but a key difference is that there is no training phase, and all the learning is done at inference time. It is therefore an instance-based approach rather than a model-based approach. Given an incomplete triple $(e_i, r_k, ?)$ we compute Concepts of Nearest Neighbours (C-NN) from the observed features of head entity e_i , where C-NNs have a representation equivalent to the bodies of AMIE+'s rules. From there, we infer a ranking of candidate entities for the tail of relation r_k . In fact, as r_k is not involved in the computation of C-NNs, many target relations can be inferred at nearly the same cost as a single relation. Indeed the main cost is in the computation of C-NNs, which is easily controlled because the computation algorithm is anytime. Compared to rule-based approaches, it

$$\begin{aligned}
E &= \{Charles, Diana, William, Harry, Kate, George, Charlotte, Louis, male, female\} \\
R &= \{parent, spouse, gender\} \\
T &= \{(\{William, Harry\}, parent, \{Charles, Diana\}), \\
&\quad (\{George, Charlotte, Louis\}, parent, \{William, Kate\}), \\
&\quad (Charles, spouse, Diana), (Diana, spouse, Charles), \\
&\quad (William, spouse, Kate), (Kate, spouse, William), \\
&\quad (\{Charles, William, Harry, George, Louis\}, gender, male), \\
&\quad (\{Diana, Kate, Charlotte\}, gender, female)\}
\end{aligned}$$

Fig. 1. Example knowledge graph describing part of the British royal family.

amounts to compute only rule bodies that match the head entity e_i , and to add the rule head according to relation r_k .

3. Preliminaries

A *knowledge graph* (KG) is defined by a structure $K = \langle E, R, T \rangle$, where E is the set of nodes, also called *entities*, R is the set of edge labels, also called *relations*, and $T \subseteq E \times R \times E$ is the set of directed and labelled edges, also called *triples*. Each triple (e_i, r_k, e_j) represents the fact that relation r_k relates entity e_i to entity e_j . This definition is very close to RDF graphs, where entities can be either URIs or literals (or blank nodes) and relations are URIs called properties. It is also equivalent to sets of logical facts, where entities are constants, and relations are binary predicates. As a running example, Figure 1 defines a small KG describing (part of) the British royal family (where $(\{a, b\}, r, \{c, d\})$ is a compact notation for (a, r, c) , (a, r, d) , (b, r, c) , (b, r, d)).

Queries based on *graph patterns* play a central role in our approach as they are used to characterize the C-NNs, and can be used as explanations for inferences. There are two kinds of *query elements*: triple patterns and filters. A *triple pattern* $(x, r, y) \in V \times R \times V$ is similar to a triple but with variables (taken from V) in place of entities. A *filter* is a Boolean expression on variables and entities. We here only consider equalities between a variable and an entity ($x = e$) and let richer filters about literal values for future work (e.g., inequalities and intervals on numbers and dates, regular expressions on strings). A *graph pattern* P is a set of query elements. $Vars(P)$ denotes the set of variables occurring in P . Equality filters are equivalent to allowing entities in triple patterns: e.g., pattern $\{(x, parent, y), (y = Kate)\}$ is equivalent to the triple pattern $(x, parent, Kate)$. There are two advantages in using filters: (1) simplifying the handling of triple patterns that have a single form (var-var) instead of four (var-var, entity-var, var-entity, entity-entity); (2) opening perspectives for richer filters (e.g., $x > 10$, $x \in [0, 10]$). A *query* $Q = (x_1, \dots, x_n) \leftarrow P$ is the projection of a graph pattern on a subset of its variables. Such queries find a concrete form in SPARQL with syntax `SELECT ?x1...?xn WHERE { P }`. Queries can be seen as anonymous rules, i.e. rules like those in AMIE+ [15] but missing the relation in the head. For example, the query $Q_{ex} = (x, y) \leftarrow (x, parent, u), (u, parent, v), (y, parent, v), (y, gender, s), (s = male)$ retrieves all (person, uncle) pairs, i.e. all pairs (x, y) where y is a sibling of a parent of x , and is male.

We now define the *answer set* that is retrieved by a query. A *matching* of a pattern P on a KG $K = \langle E, R, T \rangle$ is a mapping μ from $Vars(P)$ to entities in E such that $\mu(t) \in T$ for every triple pattern $t \in P$, and $\mu(f)$ evaluates to true for every filter $f \in P$, where $\mu(t)$ and $\mu(f)$ are obtained from t and f by

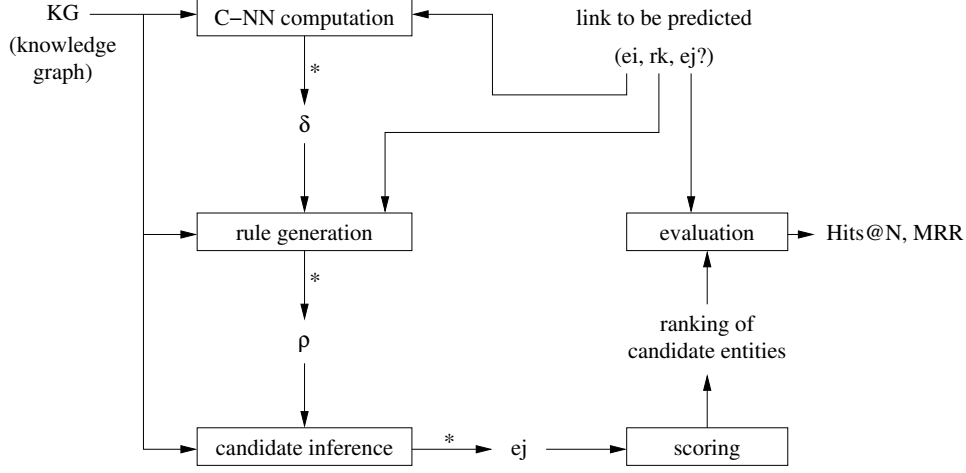


Fig. 2. Overview of link prediction based on concepts of nearest neighbours

replacing every variable x by $\mu(x)$. In the example KG, a possible matching for the pattern of the above query is $\mu_{ex} = \{x \mapsto \text{Charlotte}, y \mapsto \text{Harry}, u \mapsto \text{William}, v \mapsto \text{Diana}, s \mapsto \text{male}\}$. A matching is therefore a homomorphism from the pattern to the graph. Term “matching” is taken from the evaluation of SPARQL queries. In logics, terms “grounding” and “instantiation” are used instead. The *answer set* $ans(Q, K)$ of a query $Q = (x_1, \dots, x_n) \leftarrow P$ is the set of tuples $(\mu(x_1), \dots, \mu(x_n))$ obtained from all matchings μ of P on K . In the running example, the pair $(\text{Charlotte}, \text{Harry})$ is therefore an answer of query Q_{ex} . Note that several matchings can lead to the same answer, and that duplicate answers are ignored. In the following, we only consider queries with a single projected variable, whose sets of answers are assimilated to sets of entities.

4. Overview of the Approach

5. Concepts of Nearest Neighbours (C-NN)

In this section, we shortly recall the theoretical definitions underlying Concepts of Nearest Neighbours (C-NN), as well as the algorithmic and practical aspects of their approximate computation under a given timeout. Further details are available in [5, 6]. In the following definitions, we assume a knowledge graph $K = \langle E, R, T \rangle$.

5.1. Theoretical Definitions

Definition 1. A graph concept is defined as a pair $C = (A, Q)$, where A is a set of entities and Q is a query such that $A = ans(Q)$ is the set of answers of Q , and $Q = msq(A)$ is the most specific query that verifies $A = ans(Q)$. A is called the extension $ext(C)$ of the concept, and Q is called the intension $int(C)$ of the concept.

The most specific query $Q = msq(A)$ represents what the neighborhood of entities in A have in common. It is well-defined under graph homomorphism (unlike under subgraph isomorphism). It can be computed from A by using the categorical product of graphs (see PGP intersection \cap_q in [18]), or

equivalently Plotkin’s anti-unification of sets of facts [20]. In the example KG, William and Charlotte have in common the following query that says that they have married parents:

$$\begin{aligned} Q_{WC} &= msq(\{William, Charlotte\}) \\ &= x \leftarrow (x, gender, s), \\ &\quad (x, parent, y), (y, gender, t), (t = male), \\ &\quad (x, parent, z), (z, gender, u), (u = female), \\ &\quad (y, spouse, z), (z, spouse, y). \end{aligned}$$

We have $A_{WC} = ans(Q_{WC}) = \{William, Harry, George, Charlotte, Louis\}$ so that $C_{WC} = (A_{WC}, Q_{WC})$ is a graph concept.

A concept $C_1 = (A_1, Q_1)$ is more specific than a concept $C_2 = (A_2, Q_2)$, in notation $C_1 \leq C_2$, if $A_1 \subseteq A_2$. For example, a concept more specific than C_{WC} is the concept of *the children of Kate and William*, whose extension is $\{George, Charlotte, Louis\}$, and whose intension is

$$x \leftarrow (x, gender, s), (x, parent, y), (y = William), (x, parent, z), (z = Kate).$$

Definition 2. Let $e_1, e_2 \in E$ be two entities. The conceptual distance $\delta(e_1, e_2)$ between e_1 and e_2 is the most specific graph concept whose extension contains both entities, i.e. $\delta(e_1, e_2) = (A, Q)$ with $Q = msq(\{e_1, e_2\})$, and $A = ans(Q)$.

For example, the above concept C_{WC} is the conceptual distance between William and Charlotte. The “distance values” have therefore a symbolic representation through the concept intension Q that represents what the two entities have in common. The concept extension A contains in addition to the two entities all entities e_3 that match the common query ($e_3 \in ans(Q)$). Such an entity e_3 can be seen as “between” e_1 and e_2 : in formulas, for all $e_3 \in ext(\delta(e_1, e_2))$, $\delta(e_1, e_3) \leq \delta(e_1, e_2)$ and $\delta(e_3, e_2) \leq \delta(e_1, e_2)$. Note that order \leq on conceptual distances is a partial ordering, unlike classical distance measures.

A numerical distance $dist(e_1, e_2) = |ext(\delta(e_1, e_2))|$ can be derived from the size of the concept extension, because the closer e_1 and e_2 are, the more specific their conceptual distance is, and the smaller the extension is. For example, the numerical distance is 5 between Charlotte and William (see C_{wc}), and 3 between George and Charlotte.

Definition 3.

Table 1 lists the 6 C-NNs of Charlotte in the running example. The proper extensions of $C-NN(Charlotte, K)$ define a partition over the set of entities E , where two entities are in the same proper extension if and only if they are at the same conceptual distance to entity *Charlotte*. The intension of the associated graph concept δ_l provides a symbolic representation of the similarity between every $e' \in proper(\delta_l)$ and *Charlotte*. For instance, concept δ_2 says that *Diana* and *Kate* have in common with *Charlotte* to be female persons. Figure 3 and the last column of Table 1 give the partial ordering between C-NNs: e.g., $\delta_1 \leq \delta_2$. Smaller C-NNs contain entities that are closer to the chosen entity, here *Charlotte*. In particular, C-NNs δ_2 and δ_3 contain the nearest neighbours of *Charlotte*. Although their numerical distance are the same (3), their intensions are very different: either being female or having William and Kate as parents.

Table 1

l	$ext(\delta_l)$ (proper in bold)	$int(\delta_l)$	sub-concepts
1	{Charlotte}	$x \leftarrow (x = Charlotte)$	-
2	{Diana, Kate, Charlotte}	$x \leftarrow (x, gender, s), (s = female)$	1
3	{George, Louis, Charlotte}	$x \leftarrow (x, gender, s), (x, parent, y), (y = William),$ $(x, parent, z), (z = Kate)$	1
4	{William, Harry, <i>George, Louis, Charlotte}</i>	$x \leftarrow (x, gender, s),$ $(x, parent, y), (y, gender, t), (t = male),$ $(x, parent, z), (z, gender, u), (u = female),$ $(y, spouse, z), (z, spouse, y)$	3
5	{Charles, Diana, Kate, <i>William, Harry,</i> <i>George, Louis, Charlotte}</i>	$x \leftarrow (x, gender, s)$	2, 4
6	{female, male, ...} = E	$x \leftarrow \emptyset$	5

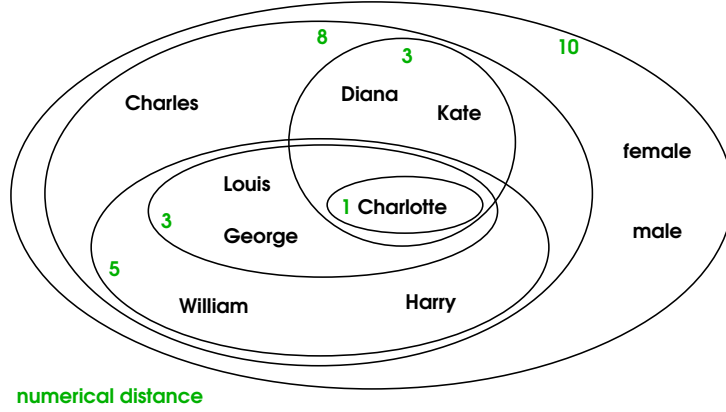


Fig. 3. Venn diagram of the extensions of the 6 C-NNs of Charlotte, labelled by their numerical distance.

Discussion. Given that $C\text{-}NN(e, K)$ partitions the set of entities, the number of C-NNs can only be smaller or equal to the number of entities, and in practice it is generally much smaller. This is interesting because, in comparison, the number of graph concepts is exponential in the number of entities in the worst case. Note that the search space of ILP approaches like AMIE+ is the set of queries, which is even larger than the set of all graph concepts. Computing the C-NNs for a given entity is therefore a much more tractable task than mining frequent patterns or learning rules, although the space of representations is the same. The pending questions that we study in this paper is whether those C-NNs are useful for inference, and how they compare to other approaches.

Compared to the use of numerical measures, like commonly done in k-NN approaches, C-NNs define a more subtle ordering of entities. First, because conceptual distances are only partially ordered, it can be that among two entities none is more similar than the other to the chosen entity e . This reflects the fact that there can be several ways to be similar to something, without necessarily a preferred one. For instance, who is most similar to Charlotte? Diana because she is also a female (C-NN δ_2) or George because he is also a son of William and Kate (C-NN δ_3)? Second, because conceptual distances partition

Algorithm 1 Partitioning algorithm for entity e in knowledge graph K

Require: $K = \langle E, R, T \rangle$ a knowledge graph, and $e \in E$ an entity

- 1: $\mathcal{S} :=$ an empty collection of clusters
- 2: $\mathcal{S}.add(E, \emptyset, descr(e))$ // the initial cluster (all entities, empty pattern, all edges describing e)
- 3: **while** no timeout $\wedge \exists (S, P, H) \in \mathcal{S} : H \neq \emptyset$ **do**
- 4: $h := chooseEdge(H)$ // choice of the splitting query element
- 5: $P_1 := P \cup \{h\}$ // refined graph pattern
- 6: $S_1 := S \cap ans(x \leftarrow P_1, K)$ // refined cluster
- 7: $S_0 := S \setminus S_1$ // remainder of cluster S
- 8: $\mathcal{S}.remove(S, P, H)$
- 9: $\mathcal{S}.add(S_1, P_1, H \setminus \{h\})$ only if $S_1 \neq \emptyset$
- 10: $\mathcal{S}.add(S_0, P, H \setminus \{h\})$ only if $S_0 \neq \emptyset$
- 11: **end while**
- 12: **return** \mathcal{S}

the set of entities, it can be said that when two entities are at the exact same conceptual distance, they are undistinguishable in terms of similarity (ex. George and Louis in C-NN δ_3). Third, the concept intension provides an intelligible explanation of the similarity to the chosen entity.

5.2. Algorithmic and Practical Aspects

We here sketch the algorithmic and practical aspects of computing the set $C-NN(e, K)$ of concepts of nearest neighbours of query entity e in a knowledge graph K . More details are available in [6]. More concretely, our algorithm works by iteratively refining a partition $\{S_i\}_i$ of the set of entities E , where each S_i is a cluster of entities, in order to get an increasingly accurate partition converging to the partition induced by the proper extensions of C-NNs.

Algorithm 1 details the partitioning algorithm. Initially, there is a single cluster $S_0 = E$ with P_0 being the empty pattern, and H_0 being the *description* of e . The description of an entity e is a graph pattern that is obtained by extracting a subgraph around e and, for each entity e_i in the subgraph, by replacing e_i by a variable y_i , and by adding filter $y_i = e_i$. Here, we choose to extract the subgraph that contains all edges starting from e up to some depth.

Then at each iteration, any cluster S – with pattern P and set of candidate query elements H – is split in two clusters S_1, S_0 by using an element $h \in H$ as a discriminating feature. Element h must be chosen so that $P \cup \{h\}$ defines a connected pattern including variable x . Each addition of a query element therefore does one of the following: (a) add a filter constraint on a pattern variable, (b) add an edge between two pattern variables, or (c) add an edge from a pattern variable to a fresh variable. Many strategies are possible for choosing this element. In this work, we only consider two simple strategies:

- **Random:** random choice among the valid elements;
- **Ordered:** choice of equality elements first, then triple patterns whose relation is the least frequently used in P (novelty).

The new clusters are defined as follows:

$$\begin{array}{llll}
 P_1 = P \cup \{h\} & Q_1 = x \leftarrow P_1 & S_1 = S \cap ans(Q_1, K) & H_1 = H \setminus \{h\} \\
 P_0 = P & Q_0 = Q & S_0 = S \setminus S_1 & H_0 = H \setminus \{h\}
 \end{array}$$

The equations for S_1, S_0 ensure that after each split there is still a partition, possibly a more accurate one. The empty clusters ($S_i = \emptyset$) are removed from the partition. As a consequence, although the search space is the set of subgraphs of the description of e , which has a size exponential in the size of the description, the number of clusters remains below the number of entities at all time. In the running example, the initial cluster S_{1-6} (the union of concepts δ_1 to δ_6) is split with element ($x = \textit{Charlotte}$) into S_1 and S_{2-6} . Then cluster S_{2-6} is split with element (x, \textit{gender}, s) into S_{2-5} and S_6 . Then cluster S_{2-5} is split with element ($s = \textit{female}$) into S_2 and S_{3-5} . Next splits involve elements (x, \textit{parent}, y) and ($y = \textit{William}$) on S_{3-5} .

Handling of RDF Schema (RDFS). The implementation takes into account the domain knowledge expressed as RDF Schema axioms [21]. A special treatment is done for triples $(e_i, \textit{rdf:type}, e_j)$, where e_j is a class, i.e. an unary predicate from the logical point of view. Such an unary predicate is simulated by not replacing e_j by a variable in the description of e . Taking inspiration from query relaxation [22], the implementation also takes into account hierarchies of classes and properties, and domains and ranges of properties. For instance, this enables to find that two entities with respective type “horse” and “cat” have type “mammal” in common, even if it does not appear in their explicit description. A naive way to achieve this is to saturate entity descriptions with inferred triples. A more efficient way is to refine the above equation defining H_0 as $H_0 = H \setminus \{h\} \cup \textit{relax}(h)$, where $\textit{relax}(h)$ is a set of relaxations of h [6]. For instance, the relaxation of a class is its set of superclasses.

Termination and efficiency. The above algorithm terminates because the set H (or its saturation in case of RDFS axioms) decreases at each split. However, in the case of large descriptions or large knowledge graphs, it can still take a long time. Now, previous experiments [6] show that most concepts are produced early, and that the rest of the time is spent at finding the last few concepts. Moreover, our algorithm is anytime because it can output a partition of entities at any time, and hence concepts of neighbours (possibly generalizations of them). It therefore makes sense to control runtime with a timeout parameter.

Actually, the above algorithm converges to an approximation of the C-NNs, in the sense that the conceptual distance may be still be an overestimate at full runtime for some entities. This is because graph patterns are constrained to be subsets of the description of e . In order to get exact results, the duplication of variables and their adjacent edges should be allowed, but this would considerably increase the search space.

Experiments on KGs with up to a million triples have shown that the algorithm can compute all C-NNs for descriptions of hundreds of edges in a matter of seconds or minutes. In contrast, query relaxation does not scale beyond 3 relaxation steps, which is insufficient to identify similar entities in most cases; and computing pairwise symbolic similarities does not scale to large numbers of entities. A key ingredient of the efficiency of the algorithm also lies in the notion of *lazy join* for the computation of answer sets of queries. In short, the principle is to compute S_1 from S in an incremental way (rather than computing $\textit{ans}(Q_1, K)$ from scratch), and to avoid the enumeration of all matchings of P_1 by computing joins only as much as necessary to compute the set of query answers (see details in [6]).

6. Link Prediction

The problem of *link prediction* is to infer a missing entity in a triple (e_i, r_k, e_j) , i.e. either infer the tail from the head and the relation, or infer the head from the tail and the relation. Because of the symmetry of the two problems, we only describe here the inference of the tail entity. In the following, we therefore consider e_i and r_k as fixed (we avoid them in indices), and e_j as variable.

6.1. C-NN-based Inference

The principle of C-NN-based inference is to generate a ruleset for each concept of neighbours $\delta_l \in C\text{-NN}(e_i, K)$. Those rules are similar in nature to those of AMIE+ or AnyBURL except that only rules that are matched by the head entity e_i are generated. Indeed, the bodies of generated rules are intensions of C-NNs, which are subsets of e_i 's description. From the concept intension $int(\delta_l) = Q_l = x \leftarrow P_l$, we generate two kinds of inference rules ρ :

- (1) **by-copy rules**: $\rho := P_l \rightarrow (x, r_k, e_j)$, for each $e_j \in E$;
- (2) **by-analogy rules**: $\rho := P_l \rightarrow (x, r_k, y)$, for each $y \in \text{Vars}(P_l), y \neq x$.

Inference by copy. The first kind of rules (**by-copy rules**) state that when an entity matches P_l as x , it is related to entity e_j through relation r_k . As e_i matches P_l as x by definition of concepts of neighbours, it can be inferred that e_i is related to e_j . Of course, the strength of the inference depends on the support and confidence of the rule ρ , which are defined as follows.

$$\text{supp}(\rho) = |\text{ans}(x \leftarrow P_l, (x, r_k, e_j))| \quad \text{conf}(\rho) = \frac{|\text{ans}(x \leftarrow P_l, (x, r_k, e_j))|}{|\text{ans}(x \leftarrow P_l)| + \lambda}$$

The support is defined as the number of entities that match P_l as x and are related to e_j through r_k . The confidence is defined as the ratio of the support out of the number of entities that match P_l as x . Like this is done in AnyBURL [17], we use a constant $\lambda \geq 0$ as a kind of additive Laplace smoothing, in order to favor rules with larger support. The principle of *inference by copy* is that the tail entities e_j to be predicted for e_i can be copied from the tail entities of e_i 's neighbour entities. For example, if triple $(\text{Charlotte}, \text{parent}, \text{Kate})$ is missing in the above example graph, it can be inferred from some of her closest neighbours: "George and Louis are similar to Charlotte because they have William as a father, and their mother is Kate, so Charlotte's mother could be Kate too" (support=2, confidence=2/(3 + λ)).

Inference by analogy. The second kind of rules (**by-analogy rules**) state that when a pair of entities match P_l as x and y , they are related through r_k . As e_i matches P_l as x by definition of concepts of neighbours, it can be inferred that e_i is related through r_k to any entity e_j that matches P_l as y when $x = e_i$. Like above, the strength of the inference depends on the support and confidence of the rule, which are defined as follows.

$$\text{supp}(\rho) = |\text{ans}((x, y) \leftarrow P_l, (x, r_k, y))| \quad \text{conf}(\rho) = \frac{|\text{ans}((x, y) \leftarrow P_l, (x, r_k, y))|}{|\text{ans}((x, y) \leftarrow P_l)| + \lambda}$$

The support is defined as the number of pairs of entities that match P_l as x and y , and that are related through r_k . The confidence is the ratio of the support out of the number of pairs of entities that match P_l as x and y , plus Laplace smoothing λ . The principle of *inference by analogy* here relies on the observation that " e_i is to e_j as x is to y ". By observing that pairs (x, y) that match pattern P_l often satisfy (x, r_k, y) , one can predict the missing entity in $(e_i, r_k, ?)$ to be any entity e_j such that pattern P_l is matched for $x = e_i$ and $y = e_j$. For example, assume in the example graph that George, Charlotte, and Louis are only known to have father William, and that Kate is only known to be William's spouse, i.e. triples $(\{\text{George}, \text{Charlotte}, \text{Louis}\}, \text{parent}, \text{Kate})$ are missing. Here, inference by copy for the parents of Charlotte would only produce Charles and Diana, using William and Harry as similar entities (see

C-NN δ_4 in Table 1). The intension of the conceptual similarity of Charlotte with William and Harry is

$$Q_{WH} = x \leftarrow P_{WH}$$

$$P_{WH} = (x, \text{gender}, s), (x, \text{parent}, y), (y, \text{gender}, t), (t = \text{male}),$$

$$(y, \text{spouse}, z), (z, \text{spouse}, y), (z, \text{gender}, u), (u = \text{female}),$$

saying that “they have a father married to a woman”. From there the following by-analogy rule can be generated: $P_{WH} \rightarrow (x, \text{parent}, z)$. This rule states that “any female spouse (wife) of a male parent (father) is a parent”. Applying this rule to Charlotte (and equivalently to George and Louis) leads to the inference of the fact $(\text{Charlotte}, \text{parent}, \text{Kate})$ because Kate is indeed the wife of William, who is the father of Charlotte. It is noteworthy here that Kate is predicted to be a parent although she never appears as a parent in the incomplete graph. This is not possible with inference by copy.

Comparison with rules in other approaches. The main difference with other rule-based approaches is that we only generate rules that are specific to the entity e_i and relation r_k for which predictions are to be made. Looking in more detail to the structure of rules, each approach has its own language bias. In AMIE+ [15], only by-analogy rules are considered, and equality filters are excluded in most experiments because they make the number of rules explodes with the length of rules. They only retain *closed* rules, i.e. rules where each variable occurs at least twice. However, non-closed rules still have to be generated in order to reach all closed rules. Another difference is about rule measures. They use *PCA confidence*, a variation of classical confidence under the *Partial Completeness Assumption (PCA)*; and *head coverage*, which is a form of recall of the rule relative to the extension of relation r_k . In AnyBURL [17], rule shapes are restricted to chains and cycles (including rule’s head), where rule’s head and equality filters cannot occur in the middle of a chain. The case of a chain with an equality filter on rule’s head is a subset of our by-copy rules. The case of a cycle is a subset of our by-analogy rules. AnyBURL supports a third kind of rule that is not covered in this work: $P \rightarrow (e_i, r_k, y)$, where $y \in \text{Vars}(P)$. Here, entities e_j are predicted based on their own description, independently of entity e_i , which acts as a constant here. In RLvLR [23], rules are equivalent to the cyclic rules of AnyBURL.

6.2. Aggregation of Inferences

Given an incomplete triple $(e_i, r_k, ?)$, the output of a link prediction system is a ranking of entities e_j . Rankings of entities are evaluated with measures such as Hits@ N (defined as 1 if the correct entity is among the first N entities, 0 otherwise), and MRR (Mean Reciprocal Rank, the inverse of the rank of the correct entity).

The question addressed in this section is how to aggregate all inferences presented in previous section into a global ranking. The same candidate e_j may be inferred by several rules, possibly generated from different concepts. In order to avoid the handling of too many rules, we exclude rules whose confidence is less than 1%, which is a very weak constraint. As a consequence, it may happen that some entities are not inferred by any rule, and hence that rankings do not include all entities of the KG. The missing entities are those for which there is not a single supporting evidence, and their rank is considered as infinite (Hits@ $N=0$, MRR=0). The idea is to combine the measures of rules to give a score to each candidate e_j , in order to get a global ranking. In this paper, we consider two scores, which we reuse or adapt from previous work, and detail below:

- **Maximum Confidence (MC)**: introduced in AnyBURL [17];
- **Dempster-Shafer (DS)**: adapted from Dencœur’s work on k-NN classification [24].

Algorithm 2 Inference and ranking of candidate entities e_j for entity e_i and relation r_k based on C-NNs

Require: $K = \langle E, R, T \rangle$ a knowledge graph, $e_i \in E$ an entity, and r_k the relation to predict for e_i

Require: $getScore$, a function computing an entity score from a set of rules (e.g., max confidence)

```

1: for all  $e_j \in E$  do
2:    $rules[e_j] := \emptyset$  // initialisation of the set of rules inferring each entity
3: end for
4: for all  $(S, P, H) \in Partitioning(e_i, K)$  // for each C-NN do
5:   for all  $e_j \in E$  do
6:      $\rho := P \rightarrow (x, r_k, e_j)$  // for each by-copy rule
7:     if  $conf(\rho) \geq minConf$  then
8:        $rules[e_j] := rules[e_j] \cup \{\rho\}$ 
9:     end if
10:  end for
11:  for all  $y \in Vars(P)$  s.t.  $y \neq x$  do
12:     $\rho := P \rightarrow (x, r_k, y)$  // for each by-analogy rule
13:    if  $conf(\rho) \geq minConf$  then
14:      for all  $e_j \in ans(y \leftarrow P, (x = e_i))$  // for each inferred entity do
15:         $rules[e_j] := rules[e_j] \cup \{\rho\}$ 
16:      end for
17:    end if
18:  end for
19: end for
20: for all  $e_j \in E$  do
21:    $score[e_j] := getScore(rules[e_j])$  // aggregating rule scores into an entity score
22: end for
23: return a ranking of entities  $e_j \in E$  according to  $score[e_j]$ 

```

Maximum Confidence (MC) score. This score is quite simple, and was shown effective in AnyBURL's work. The score of entity e_j is simply the list of the confidences of the rules that infer triple (e_i, r_k, e_j) , in decreasing order. This is a refinement of the score that was used in first experiments of AMIE, where the score was the maximum confidence among rules predicting e_j . Using a list of confidences instead of a single confidence allows for a finer ranking. Ranking of lists of confidences is done similarly to lexicographic ordering. Candidates are first compared with the first confidence. If their first confidence are equal, comparison is done with the second confidence, and so on. Then, candidates with longer lists are put first because they have more rules predicting them.

Dempster-Shafer (DS) score. This score is inspired by the work of Denœux [24], and adapted to our concepts of neighbours. Denœux defines a k-NN classification rule based on Dempster-Shafer (DS) theory. Each k -nearest neighbour x_l of an instance to be classified x is used as a piece of evidence that supports the fact that x belongs to the class c_l of x_l . The degree of support is defined as a function of the distance between x and x_l , in such a way that the choice of k is less sensitive, so that large values of k can be chosen. DS theory enables to combine the k pieces of evidence into a global evidence, and to define a measure of *belief* for each class, which can be used as a score.

We adapt Denœux's work to the inference of e_j in triple $(e_i, r_k, ?)$ in the following way. Each rule ρ that predicts e_j is used as a piece of evidence. The degree of support depends on the extensional dis-

tance $dist(\rho) = |ext(\delta_l)|$ of the concept of neighbours δ_l that generated the rule, and on the confidence of the rule. In order to have comparable pieces of evidence, we instantiate each by-analogy rule $P_l \rightarrow (x, r_k, y)$ for each possible value of y into a by-copy rule: $P_l, (y = e_j) \rightarrow (x, r_k, e_j)$. Indeed, by-analogy rules tend to be more general, and hence to have larger distances.

Because in KGs a head entity can be linked to several tail entities through the same relation, we consider a distinct classification problem for each candidate tail entity $e_j \in E$ with two classes c_j^1 (e_j is a tail entity) and c_j^0 (e_j is not a tail entity). For each candidate entity e_j and each rule ρ predicting e_j , the degree of support can therefore be formalized by defining a mass distribution $m_{j,\rho}$ over sets of classes as follows.

$$m_{j,\rho}(\{c_j^1\}) = \alpha_0 \text{conf}(\rho) e^{-dist(\rho)} \quad m_{j,\rho}(\{c_j^0\}) = 0 \quad m_{j,\rho}(\{c_j^1, c_j^0\}) = 1 - \alpha_0 \text{conf}(\rho) e^{-dist(\rho)}$$

$m_{j,\rho}(\{c_j^1\})$ represents the degree of belief for e_j being the tail entity, while $m_{j,\rho}(\{c_j^1, c_j^0\})$ represents the degree of uncertainty. $m_{j,\rho}(\{c_j^0\})$ is set to 0 to reflect the OWA (Open World Assumption) of KGs according to which a missing fact is not considered as false. Constant α_0 determines the maximum degree of belief, which can be lower than 1 to reflect uncertainty about known triples (e.g. 0.95). The degree of belief decreases exponentially with distance. Finally, we make the degree of belief proportional to the confidence of inferring entity e_j with rule ρ . In [24], that confidence factor does not exist because it would be 1 for the class of the nearest neighbour, and 0 for every other class.

By applying Dempster-Shafer theory to combine the evidence from all rules ρ that predict entity e_j , we arrive at the following equation for the belief of each candidate tail entity e_j .

$$Bel_j = m_j(\{c_j^1\}) = 1 - \prod_{\rho} 1 - \alpha_0 \text{conf}(\rho) e^{-dist(\rho)}$$

We can use that belief as a score to rank all predicted entities by decreasing belief. The score used by AMIE+ is a special case of this score, where $\alpha_0 = 1$, $dist(\rho) = 0$ for all rules, and PCA confidence is used instead of classical confidence.

6.3. Inference Algorithm and Explanations

7. Experiments

We here report on experiments comparing our approach to other approaches on several standard benchmarks for link prediction. We first present the methodology, and study the impact on performance of the different strategies and hyper-parameters of our approach. Then we report performance results on benchmarks with an in-depth analysis, and finally present a fine-grained comparison with AnyBURL. The companion page² provides access to the source code, the datasets, and the experiment main results and logs.

7.1. Methodology

Datasets. We use four datasets that are used in many work to evaluate the link prediction task (WN18, WN18RR, FB15k, FB15k-237), plus an additional dataset that we derived from the Mondial dataset [25].

²Companion page: http://www.irisa.fr/LIS/ferre/pub/link_prediction2020/

Table 2
Statistics of datasets.

Dataset	entities	relations	train edges	valid. edges	test edges
WN18	40 943	18	141 442	5 000	5 000
WN18RR	40 559	11	86 835	3 034	3 134
FB15k	14 951	1 345	483 142	50 000	59 071
FB15k-237	15 541	237	272 115	17 535	20,466
Mondial	2 473	20	8 456	570	701

Table 2 provides statistics about datasets (numbers of: entities, relations, train edges, validation edges, and test edges). WN18 and FB15k were introduced by Bordes *et al* [7] for link prediction evaluation. WN18 is derived from a subset of WordNet, and FB15k from FreeBase. In later work, it was observed that many test triples had their inverse in the training set (e.g., *hypernym* is the inverse of *hyponym* in WordNet), and could be solved with very simple rules (e.g., $(y, \textit{hypernym}, x) \rightarrow (x, \textit{hyponym}, y)$). More challenging datasets were introduced by removing from the validation and test sets all pairs of entities that occur in the training set. FB15k-237 was introduced by Toutanova and Chen [8], and WN18RR was introduced by Dettmers *et al.* [9].

We introduce Mondial as a subset of the Mondial database [25], which contains facts about world geography. We simplified it to the task of link prediction by removing labelling edges and edges containing dates and numbers, and by unreifying n-ary relations into binary relations. Triples whose relation is `rdf:type` were also removed from the validation and test sets because they do not represent proper links between entities. The dataset is available from the companion page. It is smaller than other datasets but it makes it easier to interpret results, and we use it to study the impact of the different strategies and hyper-parameters without introducing a bias in our evaluation on the classical benchmarks.

Task. We follow the same protocol as introduced in [7], and followed by subsequent work. The task is to infer, for each test triple, the tail entity from the head and the relation, and also the head entity from the tail and the relation. We call *test entity* the known entity, and *missing entity* the entity to be inferred. We evaluate the performance of our approach by using the same three measures as in [17]: MRR and Hits@{1,10} (given in percents in this paper). Like in previous work, we use filtered versions of those measures to reflect the fact that, for instance, there may be several correct tail entities for a 1-n relation (e.g., the relation from awards to nominees). For example, if the correct entity is at rank 7 but 2 out of the first 6 entities form triples that belong to the dataset (and are therefore considered as valid), then it is considered to be at rank 5.

Method. Because our approach has no training phase we can use both train and validation datasets as examples for our instance-based inference. We consider a few alternative strategies:

- Random vs Ordered choice of a query element in the partitioning algorithm (see Section 5.2);
- by-copy vs by-analogy vs both kinds of inference rules (see Section 6.1);
- MC vs DS score for ranking inferred entities (see Section 6.2).

Our approach has only three hyper-parameters (and no parameter to learn): the *maximum depth* of the description of the test entity, and two *timeouts*: one for the computation of C-NNs, and another one for the inference of an entity ranking. For the inference of a ranking of entities, we set $\lambda = 2$ in the definition of rule confidence, and $\alpha_0 = 0.95$ in the DS-score.

The implementation of our approach has been integrated to SEWELIS as an improvement of previous work on the guided edition of RDF graphs [26]. A standalone program for link prediction is available

Table 3
Comparing MRR on Mondial with 12 different strategies

	by-copy		by-analogy		by-copy+analogy	
	MC	DS	MC	DS	MC	DS
Random	28.6	16.9	42.4	41.3	45.5	44.2
Ordered	30.1	19.2	33.7	30.8	40.2	37.3

from the companion page. We ran our experiments on Fedora 25, with CPU Intel(R) Core(TM) i7-6600U @ 2.60GHz, and 16GB DDR4 memory. So far, our implementation is simple and uses a single core, although our partitioning algorithm lends itself to parallelization. We have observed that in all our experiments the memory footprint, which includes the training and validation triples, remains under a few percents, i.e. a few hundreds MB. An alternative implementation³ for the computation of C-NNs has recently been developed as a Java library on top of the Jena Framework⁴, in order to facilitate their reuse in other applications.

Baselines. We compare our approach to a number of historical or state-of-the-art latent-based approaches: DISTMULT [27], ANALOGY [28], KB_LR [29], R-GCN+ [10], ConvE [9], ComplEx-N3 [11], and CrossE [30]. We do so by choosing the same tasks and measures as in previous work because it was not possible for us to run them ourselves (no access to a GPU), and also because it allows for a fairer comparison (e.g., choice of hyper-parameters by authors). We also compare our approach to rule-based approaches: AMIE+ [15], RuleN [16], and AnyBURL [17]. Most performance results of the above approaches are reproduced from Meilicke *et al.* [17] (see Section 7.3 for details). We add yet another baseline *Freq* that simply consists in ranking entities e_j according to their decreasing frequency of usage in r_k over the train+valid dataset, as defined by $freq_j = |ans(x \leftarrow (x, r_k, y), (y = e_j))|$. It is independent of the test entity, and therefore acts as a default ranking.

7.2. Impact of Strategies and Hyper-parameters and Consistency of Results

Impact of strategies. Table 3 compares the obtained MRR (in percents) on the Mondial dataset with different strategies. The timeout was set to 0.1s for both C-NN computation and inference, and the maximum depth was set to 3. For recall, there are three axes composing the strategy:

- choice of a splitting element: **Random** vs **Ordered**;
- kinds of inference rules: **by-copy** vs **by-analogy** vs both (**by-copy+analogy**);
- aggregation of inferences: **MC** (max. confidence) vs **DS** (Dempster-Shafer).

This results in 12 different strategies, and Table 3 shows that the best performing combines **Random**, **by-copy+analogy**, and **MC**. Looking more in detail, we observe that combining both kinds of rules is always beneficial, as well as aggregating inferences with maximum confidence. However, **Ordered** element choice is better with **by-copy** rules, while **Random** element choice is better with **by-analogy** rules. We can also evaluate the importance of each axis by measuring the MRR decrease when replacing the best option by another. The most important options are in order: **by-analogy** rules (-16.9), **Random** choice (-5.3), **by-copy** rules (-3.1), and finally **MC** aggregation (-1.3). From now on, we only use the best performing strategy.

³<https://bitbucket.org/sebferre/conceptsofneighbours/>

⁴<https://jena.apache.org/>

Table 4
Evolution of performance and internal parameters with timeout

timeout(s)	Hits@1	Hits@10	MRR	nb. concepts	nb. inferred	max. conf
0.001	15.7	31.8	21.2	3.7	103	0.20
0.01	32.3	51.3	38.9	11.9	211	0.42
0.1	38.6	59.1	45.5	35.0	311	0.57
1	39.3	63.7	47.3	89.2	351	0.66

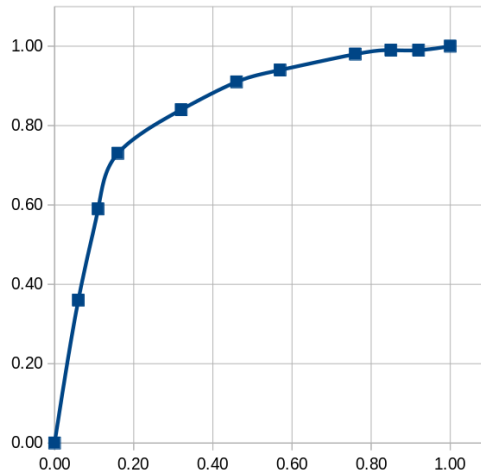


Fig. 4. ROC curve of predicting Hits@1 correctness depending on maximum confidence threshold

Impact of timeout. Table 4 shows the evolution of a number of measures when timeout exponentially increases from 1ms to 1s. There are three performance measures (Hits@1, Hits@10, MRR), followed by three measures about the inference process, averaged over the test set: number of computed concepts of neighbours, number of inferred entities, and maximum confidence over all inferred entities. It can be observed that with only 1% of the largest timeout (timeout 0.01s vs 1s), the MRR is already at 82% of the larger MRR, and 60% of the inferred entities are obtained, despite the fact that only 13% of the concepts have been computed. This indicates that early approximations of concepts of neighbours are already informative. Furthermore, increasing the timeout and hence the number of concepts does not only improve MRR but also increases confidence in inferences as indicated by the steadily increasing maximum confidence.

Impact of description depth. We have observed that increasing description depth beyond 2-3 makes almost no significant difference on performance measures, as well as on the number of inferred entities and on the maximum confidence. In the following, we therefore stick to a maximum description depth equal to 3.

Consistency of results. To evaluate the consistency of the results of our approach, we perform two analyses on the Mondial dataset (with timeout=0.1s). First, we analyze the variability of the performance measures by splitting the test set 10-fold. We observe that the standard error across the 10 folds is very small for all measures: e.g., 0.5% for MRR, around 1% for Hits@1 and Hits@10, and 0.4% for maximum confidence.

Table 5
Comparison of performance results on WN18 and WN18RR

Approach	source	WN18			WN18RR		
		H@1	H@10	MRR	H@1	H@10	MRR
<i>Freq</i>		1.8	5.0	2.9	1.5	4.4	2.6
<i>Latent-based</i>							
DISTMULT [27]	[10]	70.1	94.3	81.3	-	-	-
ANALOGY [28]	[28]	93.9	-	94.2	-	-	-
KB_LR [29]	[29]	-	95.1	93.6	-	-	-
R-GCN+ [10]	[17]	69.7	96.4	81.9	-	-	-
ConvE [9]	[17]	93.5	95.5	94.2	39.0	48.0	46.0
ComplEx-N3 [11]	[17]	-	96.0	95.0	-	57.0	48.0
CrossE [30]	[17]	74.1	95.0	83.0	-	-	-
<i>Rule-based</i>							
AMIE+ [15]	[17]	87.2	94.8	-	35.8	38.8	-
RuleN [16]	[17]	94.5	95.8	-	42.7	53.6	-
AnyBURL [17]	[17]	93.9	95.6	95.0	44.6	55.5	48.0
C-NN (ours)		96.7	97.2	96.9	44.4	51.9	46.9
C-NN – best other		+2.2	+0.8	+1.9	-0.2	-5.1	-1.1
C-NN – best other rule-based		+2.2	+1.4	+1.9	-0.2	-3.6	-1.1

Second, we analyze the relevance of the maximum confidence by measuring how predictive it is about the correctness of predictions. Figure 4 shows the ROC curve for the classification task that consists in predicting whether the top entity in the filtered ranking is correct based on the hypothesis that its associated maximum confidence is above a threshold varying from 0 to 1. For example, with threshold at 0.70, the true positive rate is at 73% while the false positive rate is at 16%. The shape of the curve, as well as its AUC (Area Under Curve) equal to 84%, demonstrate the relevance of the maximum confidence to estimate the validity of predictions. This comes in complement with interpretable explanations for inferred entities in the form of rules.

7.3. Results on Benchmarks

Tables 5 and 6 compare the results of our approach (C-NN) to other approaches presented above as baselines on the four datasets WN18, WN18RR, FB15k, and FB15k-237. The baselines are organized in three groups: naive baseline *Freq*, latent-based approaches, and rule-based approaches. In each group, approaches are sorted by publication year. The *source* indicates which paper the results are taken from. The results for AnyBURL are those where 1000s (largest available time) are allocated to the computation of rules. In the results of C-NN, the timeouts (computation of concepts + inference) are 1+1s for WN datasets, and 1.5+0.5s for FB datasets. The output logs of C-NN predictions and explanations are available from the companion page.

ComplEx-N3 clearly outperforms other approaches on all datasets except WN18 where C-NN outperforms other approaches on the three measures. C-NN comes second on FB15k, and remains close to the best approaches on WN18RR. On FB15k-237, the MRR delta is -7.4 with ComplEx-N3, but only -0.4 with AnyBURL, the best rule-based approach. It is noteworthy that C-NN is competitive with AnyBURL because, whereas AnyBURL rules are computed in a supervised manner (knowing the target relation r_k), C-NN concepts are computed in an unsupervised manner (i.e, only knowing the source entity e_i). This

Table 6
Comparison of performance results on FB15k and FB15k-237

Approach	source	FB15k			FB15k-237		
		H@1	H@10	MRR	H@1	H@10	MRR
<i>Freq</i>		14.3	28.5	19.2	17.5	35.6	23.6
<i>Latent-based</i>							
DISTMULT [27]	[10]	52.2	81.4	63.4	10.6	37.6	19.1
ANALOGY [28]	[28]	64.6	-	72.5	-	-	-
KB_LR [29]	[29]	74.2	87.3	79.0	22.0	48.2	30.6
R-GCN+ [10]	[17]	60.1	84.2	69.6	15.1	41.7	24.9
ConvE [9]	[17]	67.0	87.3	74.5	23.9	49.1	31.6
ComplEx-N3 [11]	[17]	-	91.0	86.0	-	56.0	37.0
CrossE [30]	[17]	63.4	87.5	72.8	21.1	47.4	29.9
<i>Rule-based</i>							
AMIE+ [15]	[17]	64.7	85.8	-	17.4	40.9	-
RuleN [16]	[17]	77.2	87.0	-	18.2	42.0	-
AnyBURL [17]	[17]	80.4	89.0	83.0	23.0	47.9	30.0
C-NN (ours)		82.7	89.0	84.9	22.2	44.6	29.6
C-NN – best other		+2.3	-2.0	-1.1	-1.7	-11.4	-7.4
C-NN – best other rule-based		+2.3	0.0	+1.9	-0.8	-3.3	-0.4

Table 7
Split of test sets depending on the kind of inference rule (by-copy vs by-analogy).

measure	WN18		WN18RR		FB15k		Fb15k-237	
	by-c	by-a	by-c	by-a	by-c	by-a	by-c	by-a
percent	2%	98%	38%	57%	14%	85%	73%	25%
Hits@1	15.0	98.7	15.2	67.8	37.0	91.0	26.2	12.2
Hits@10	34.4	98.8	29.4	71.6	63.5	94.2	49.9	32.3
MRR	22.0	98.7	19.9	69.1	47.0	92.1	34.1	18.7
max. conf	0.24	0.96	0.28	0.70	0.60	0.88	0.61	0.66

implies that the concepts of neighbours of an entity can be computed once, and used for many different inference tasks, e.g. predicting links for several target relations.

Looking at the *Freq* baseline, it becomes visible how FB15k-237 is difficult because performance improvements over *Freq* are relatively small while they are huge on other datasets.

7.4. In-depth Analysis of Results

In this section, we refine the performance evaluation of our approach by analysing results w.r.t two criteria: (a) the kind of rule (by-copy vs by-analogy) that inferred the rank-1 predictions, (b) the characteristics of the relation to be predicted.

Prediction by-copy vs by-analogy. We here analyze predictions according to the kind of the *best rule*, i.e. the rule with highest confidence, which contributed to decide the first entity in the generated ranking. For recall, there are two kinds of rules: by-copy rules and by-analogy rules (see Section 6.1). Table 7 shows the performance measures, and maximum confidence, on two subsets of the test set for each dataset, depending on the kind of the best rule. Line “percent” gives the relative size of those subsets.

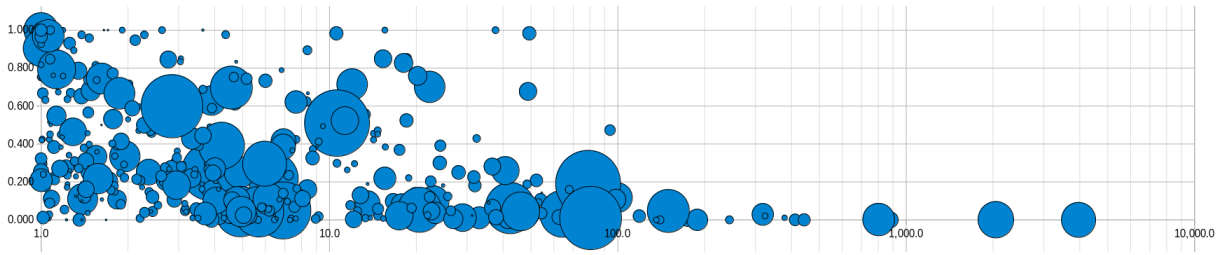


Fig. 5. MRR as a function of relation degree. Bubble sizes are proportional to relation frequency.

The two percentages may not sum up to 100% because for some test cases, no prediction could be made: e.g., all predicted entities are already known to hold, and are therefore filtered out.

The balance between by-copy and by-analogy can be explained by the nature of each dataset. In WN18 and FB15k it is well known that most test triples can be inferred from an inverse triple, which is well captured with by-analogy rules: e.g., $hypernym(y, x) \rightarrow hyponym(x, y)$. In FB15k-237, all inverse triples have been removed, and for many relations, some candidate entities are much more frequent than others: e.g., US nationality for people. Those frequent entities are easily inferred with by-copy rules. In WN18RR, by-analogy rules remain dominant for two reasons. First, inverse relations have been removed (e.g., $hyponym$ as inverse of $hypernym$), but other inverse triples have been retained. In particular, symmetric relations such as *similar_to* and *derivationally_related_form* are still present, and account for about one third of test triples. Second, there are much less situations like “US nationality”, where a single word would dominate in a relation. The performance measures (Hits@1, Hits@10, MRR) are consistent with the balance between by-copy and by-analogy: measures are better for the most frequent kind of rule. However, it appears that by-analogy rules always have a higher confidence on average. We hypothesize that this is because by-analogy inference relies on the similarity with not only entity e_i but with pair of entities (e_i, e_j) , and involves an explicit relationship between e_i and e_j , expressed as a graph pattern.

Results depending on relation characteristics. Relations are not all alike in knowledge graphs. They vary in frequency, and whether they are functional or multi-valued. We here define the *frequency* of a relation r as the number of test triples using it; and its *degree* as the average number of tail entities per head entity in the training set. When the degree equals (or is closed to) 1, the relation is said *functional*, otherwise it is said *multi-valued*. As the benchmarks imply to predict both the tail from the head, and the head from the tail, we also consider inverse relations. Their frequency is the same, and their degree is the average number of head entities per tail entity. The degree of the inverse relation is unrelated to the degree of the relation, and all combinations are possible, i.e. 1-1, n-1, 1-n, and n-n relations.

Figure 5 shows a bubble plot of the 224 relations and their inverses, which are found in the test set of FB15k-237, the most challenging dataset. Each bubble is positioned according to its degree (ranging from 1 to 4000), and to the MRR of its predictions (ranging from 0 to 1). The bubble size reflects the frequency of the relation, and hence its weight in the global performance measures. Several observations can be made. First, the relations cover a wide range of frequencies and degrees, and there are no obvious correlation between those two dimensions. Second, there is a clear tendency that the higher the degree, the lower the MRR, i.e. multi-valued relations are harder to predict than functional relations. However, many relations stand under and above this tendency. Some relations have a low MRR despite a low degree (e.g., *place of birth*); and some relation succeeds to have a high MRR despite degrees up to 50 (e.g.,

Table 8

Distribution of test instances depending of Hits@1 success of C-NN and AnyBURL. The last two columns give the average Hits@1 first for the best of the two approaches, and second for the best ensemble.

dataset	nb. test	H@1 C-NN / H@1 AnyBURL				H@1	
		1 / 1	1 / 0	0 / 1	0 / 0	best of two	best ensemble
WN18	10 100	93.2	3.4	0.9	2.5	96.6	97.5
WN18RR	6 268	41.3	3.1	3.6	52.0	44.9	48.0
FB15k	118 142	75.3	7.4	5.5	11.8	82.7	88.2
FB15k-237	40 932	17.5	4.7	6.2	71.6	23.7	28.4

inverse of *food nutrient* with degree=15). Examples of frequent relations with high MRR are: *people nationality* (degree=1.1, MRR=79.3), *people gender* (degree=1, MRR=90.4), *topic webpage category* (degree=1, MRR=100), *marriage type of union* (degree=1.1, MRR=100), *award winners ceremony* (degree=12, MRR=71.4), and its inverse (degree=22, MRR=70.1).

7.5. Detailed Comparison with AnyBURL

In this section, we detail the comparison with predictions made by AnyBURL⁵. Indeed, AnyBURL is the state-of-the-art among rule-based approaches. The main question we answer here is: How predictions differ between C-NN and AnyBURL. Table 8 gives for the four datasets the distribution of test instances into four cases depending on the Hits@1 success of each approach (C-NN and AnyBURL). If the rank-1 predicted entity is correct, then Hits@1 equals 1, otherwise it equals 0. Case 1/1 means that both approaches are correct, case 1/0 means that C-NN is correct but not AnyBURL, etc. The four cases sum up to 100%.

We consider the null hypothesis that if one approach has lesser performance, then its set of correct predictions is a subset of the correct predictions of the other approach. For instance, on FB15k-237 where AnyBURL is better, we expect that case 0/1 is empty. This is contradicted in all four datasets. For instance, on FB15k-237, C-NN is the only correct approach for 4.7% test instances, which amounts to 1918 test instances. Those results demonstrate that C-NN and AnyBURL can complement each other, and that improvement of state-of-the-art performances remains possible. This is made explicit in the last two columns that allow to compare Hits@1 of the best of the two approaches and the best ensemble of the two (union of correct predictions).

We now detail a few test instances where C-NN and AnyBURL differ (cases 1/0 and 0/1). The analysis is limited by the fact that AnyBURL’s code does not output rules as explanations for predictions (although the code could be modified to do so). Here are a few test instances where C-NN succeeds while AnyBURL fails:

- Wichita falls were correctly predicted to have Central Time Zone because it is contained in Texas (by-copy rule, support=31, confidence=0.79);
- Joe Shuster was correctly predicted to have written “Superman II: The Richard Donner Cut” because he has produced a story that was honored for the film, and he won some award (by-analogy rule, support=5, confidence=0.36);
- Joe Shuster was also correctly predicted to live in Cleveland because he has produced the story “Superman II” (by-copy rule, support=1, confidence=0.33);

⁵Detailed predictions for state-of-the-art latent-based approaches are not available, and specific hardware (GPUs) is required to run them in a reasonable amount of time.

- Film “Good Will Hunting” was correctly predicted to have two crew roles “make-up artist” and “special effects supervisor” because it was nominated for the “Satellite Award for Best Original Screenplay” (by-copy rule, support=16, confidence=0.78).

Those C-NN rules could be found by AnyBURL, so they do not exhibit real limits of AnyBURL. However, all those rules except the second contain equality filters (constants in AnyBURL’s terminology), and the number of such rules is extremely large, even for small rules, because of the high number of entities in KGs. C-NN here has the advantage that it only needs to generate rules for a given test instance (instance-based learning), while AnyBURL has to generate the rules before seeing any test instance (model-based learning). We can therefore expect C-NN to have a better coverage of such rules.

Now, here are test instances where C-NN fails while AnyBURL succeeds. In each instance, we give the best C-NN rule, which fails, and then the “successful C-NN rule”, i.e. the highest-confidence rule found by our approach that infer the correct entity.

- Lily Tomlin was incorrectly predicted to be nominated for TV series “Murphy Brown”, instead of “The West Wing” (predicted 2nd), because he is an actor of the TV series, and won an award (by-analogy rule, support=364, confidence=0.53). The successful rule predicts “The West Wing” because he was nominated along with Joshua Malina (by-copy rule, support=14, confidence=0.50);
- Film “Life is beautiful” was incorrectly predicted to have genre Italian, instead of War Film (predicted 8th), because it appears on the title list of the Netflix genre “Italian” (by-analogy rule, support=393, confidence=0.56). The successful rule predicts War Film because it was produced in Italy (by-copy rule, support=14, confidence=0.25).

It is difficult to derive conclusions without knowing the successful AnyBURL’s rules. Still, it can be observed that errors made by C-NN are reasonable ones. In the second example, the successful rule has weaker measures of support and confidence, and is less intuitive than the unsuccessful one. In reality, the film “Life is beautiful” has both genres “Italian” and “War Film”, but the gold standard only contains the second. One must keep in mind that what is used as gold standard in those experiments are actually incomplete (and possibly incorrect) knowledge graphs.

8. Conclusion

We have shown that a symbolic approach to the problem of knowledge graph completion can be competitive with state-of-the-art approaches, both latent-based and rule-based. This comes with the major advantage that our approach can provide detailed explanations for each inference, in terms of the graph features. Compared to rule-based approaches, which can provide similar explanations, we avoid the need for a training phase that can be costly in runtime and memory (rule mining), in particular with dynamic data. Our approach is analogous to classification with k-nearest neighbours but our distances are defined as partially-ordered graph concepts instead of numbers.

There are many tracks for future work. Extending graph patterns with n-ary relations and richer filters over numbers, dates, etc. Optimizing the computation of C-NNs by finding good strategies to drive the partitioning process, or by parallelizing it. Evaluating our approach on other datasets, and other inference tasks.

References

- [1] S. Ferré, Link Prediction in Knowledge Graphs with Concepts of Nearest Neighbours, in: *The Semantic Web (ESWC)*, P. Hitzler et al., eds, LNCS 11503, Springer, 2019, pp. 84–100. doi:10.1007/978-3-030-21348-0_6.
- [2] T. Berners-Lee, J. Hendler and O. Lassila, The Semantic Web, *Scientific American* **284**(5) (2001), 34–43.
- [3] M. Nickel, K. Murphy, V. Tresp and E. Gabrilovich, A review of relational machine learning for knowledge graphs, *Proc. IEEE* **104**(1) (2016), 11–33.
- [4] D. Liben-Nowell and J. Kleinberg, The link-prediction problem for social networks, *Journal of the American society for information science and technology* **58**(7) (2007), 1019–1031.
- [5] S. Ferré, Concepts de plus proches voisins dans des graphes de connaissances, in: *Ingénierie des Connaissances (IC)*, 2017, pp. 163–174.
- [6] S. Ferré, Answers Partitioning and Lazy Joins for Efficient Query Relaxation and Application to Similarity Search, in: *Int. Conf. The Semantic Web (ESWC)*, A. Gangemi et al., eds, LNCS 10843, Springer, 2018, pp. 209–224. doi:10.1007/978-3-319-93417-4_14.
- [7] A. Bordes, N. Usunier, A. Garcia-Duran, J. Weston and O. Yakhnenko, Translating embeddings for modeling multi-relational data, in: *Advances in neural information processing systems*, 2013, pp. 2787–2795.
- [8] K. Toutanova and D. Chen, Observed versus latent features for knowledge base and text inference, in: *Work. Continuous Vector Space Models and their Compositionality*, 2015, pp. 57–66.
- [9] T. Dettmers, P. Minervini, P. Stenetorp and S. Riedel, Convolutional 2D Knowledge Graph Embeddings, in: *Conf. Artificial Intelligence (AAAI)*, S.A. McIlraith and K.Q. Weinberger, eds, AAAI Press, 2018, pp. 1811–1818.
- [10] M. Schlichtkrull, T.N. Kipf, P. Bloem, R. van den Berg, I. Titov and M. Welling, Modeling relational data with graph convolutional networks, in: *The Semantic Web Conf. (ESWC)*, Springer, 2018, pp. 593–607.
- [11] T. Lacroix, N. Usunier and G. Obozinski, Canonical Tensor Decomposition for Knowledge Base Completion, in: *Int. Conf. Machine Learning*, J.G. Dy and A. Krause, eds, Proceedings of Machine Learning Research, Vol. 80, PMLR, 2018, pp. 2869–2878. <http://proceedings.mlr.press/v80/lacroix18a.html>.
- [12] R. Zhang, J. Li, J. Mei and Y. Mao, Scalable Instance Reconstruction in Knowledge Bases via Relatedness Affiliated Embedding, in: *Conf. World Wide Web (WWW)*, 2018, pp. 1185–1194.
- [13] N. Lao, T. Mitchell and W.W. Cohen, Random walk inference and learning in a large scale knowledge base, in: *Conf. Empirical Methods in Natural Language Processing*, Association for Computational Linguistics, 2011, pp. 529–539.
- [14] S. Muggleton, Inverse Entailment and Progol, *New Generation Computation* **13** (1995), 245–286.
- [15] L. Galárraga, C. Teflioudi, K. Hose and F. Suchanek, Fast rule mining in ontological knowledge bases with AMIE+, *Int. J. Very Large Data Bases* **24**(6) (2015), 707–730.
- [16] C. Meilicke, M. Fink, Y. Wang, D. Ruffinelli, R. Gemulla and H. Stuckenschmidt, Fine-Grained Evaluation of Rule- and Embedding-Based Systems for Knowledge Graph Completion, in: *The Semantic Web (ISWC)*, D. Vrandečić et al., eds, LNCS 11136, Springer, 2018, pp. 3–20. doi:10.1007/978-3-030-00671-6_1.
- [17] C. Meilicke, M.W. Chekol, D. Ruffinelli and H. Stuckenschmidt, Anytime Bottom-Up Rule Learning for Knowledge Graph Completion, in: *Int. Joint Conf. Artificial Intelligence (IJCAI)*, S. Kraus, ed., ijcai.org, 2019, pp. 3137–3143. doi:10.24963/ijcai.2019/435.
- [18] S. Ferré and P. Cellier, Graph-FCA: An extension of formal concept analysis to knowledge graphs, *Discrete Applied Mathematics* **273** (2019), 81–102. doi:<https://doi.org/10.1016/j.dam.2019.03.003>. <http://www.sciencedirect.com/science/article/pii/S0166218X19301532>.
- [19] B. Ganter and R. Wille, *Formal Concept Analysis — Mathematical Foundations*, Springer, 1999.
- [20] G.D. Plotkin, Automatic Methods of Inductive Inference, PhD thesis, Edinburgh University, 1971.
- [21] P. Hitzler, M. Krötzsch and S. Rudolph, *Foundations of Semantic Web Technologies*, Chapman & Hall/CRC, 2009. ISBN 9781420090505.
- [22] C.A. Hurtado, A. Poulouvasilis and P.T. Wood, Query Relaxation in RDF, in: *Journal on Data Semantics X*, S. Spaccapietra, ed., LNCS 4900, Springer, 2008, pp. 31–61.
- [23] P.G. Omran, K. Wang and Z. Wang, Scalable Rule Learning via Learning Representation, in: *Int. Joint Conf. Artificial Intelligence (IJCAI)*, J. Lang, ed., ijcai.org, 2018, pp. 2149–2155. doi:10.24963/ijcai.2018/297.
- [24] T. Denœux, A k-nearest neighbor classification rule based on Dempster-Shafer theory, *IEEE Trans. Systems, Man, and Cybernetics* **25**(5) (1995), 804–813.
- [25] W. May, Information Extraction and Integration with FLORID: The MONDIAL Case Study, Technical Report, 131, Universität Freiburg, Institut für Informatik, 1999, Available from <http://dbis.informatik.uni-goettingen.de/Mondial>.
- [26] A. Hermann, S. Ferré and M. Ducassé, An Interactive Guidance Process Supporting Consistent Updates of RDFS Graphs, in: *Int. Conf. Knowledge Engineering and Knowledge Management (EKAW)*, A. ten Teije et al., eds, LNAI 7603, Springer, 2012, pp. 185–199.
- [27] B. Yang, W. Yih, X. He, J. Gao and L. Deng, Embedding Entities and Relations for Learning and Inference in Knowledge Bases, in: *Int. Conf. Learning Representations (ICLR)*, Y. Bengio and Y. LeCun, eds, 2015. <http://arxiv.org/abs/1412.6575>.

- 1 [28] H. Liu, Y. Wu and Y. Yang, Analogical Inference for Multi-relational Embeddings, in: *Int. Conf. Machine Learning (ICML)*, D. Precup and Y.W. Teh, eds, Proceedings of Machine Learning Research, Vol. 70, PMLR, 2017, pp. 2168–2178. 1
2 <http://proceedings.mlr.press/v70/liu17d.html>. 2
- 3 [29] A. García-Durán and M. Niepert, KBIn: End-to-End Learning of Knowledge Base Representations with Latent, Rela- 3
4 tional, and Numerical Features, in: *Conf. Uncertainty in Artificial Intelligence (UAI)*, A. Globerson and R. Silva, eds, 4
5 AUAI Press, 2018, pp. 372–381. <http://auai.org/uai2018/proceedings/papers/149.pdf>. 5
- 6 [30] W. Zhang, B. Paudel, W. Zhang, A. Bernstein and H. Chen, Interaction Embeddings for Prediction and Explanation in 6
7 Knowledge Graphs, in: *Int. Conf. Web Search and Data Mining (WSDM)*, J.S. Culpepper, A. Moffat, P.N. Bennett and 7
8 K. Lerman, eds, ACM, 2019, pp. 96–104. doi:10.1145/3289600.3291014. 8
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