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Neural axiom network for knowledge graph reasoning

Juan Li a,*, Xiangnan Chen a, Hongtao Yu a, Jiaoyan Chen b and Wen Zhang c,*,**

E-mails: lijuan18@zju.edu.cn, xnchen2020@zju.edu.cn, yuhongtaoaaa@zju.edu.cn

E-mail: jiaoyan.chen@cs.ox.ac.uk

E-mail: zhang.wen@zju.edu.cn

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Abstract. Knowledge graph reasoning (KGR) aims to infer new knowledge or detect noises, which is essential for improving the quality of knowledge graphs. Recently, various KGR techniques, such as symbolic- and embedding-based methods, have been proposed and shown strong reasoning ability. Symbolic-based reasoning methods infer missing triples according to predefined rules or ontologies. Although rules and axioms have proven effective, it is difficult to obtain them. Embedding-based reasoning methods represent entities and relations as vectors, and complete KGs via vector computation. However, they mainly rely on structural information and ignore implicit axiom information not predefined in KGs but can be reflected in data. That is, each correct triple is also a logically consistent triple and satisfies all axioms. In this paper, we propose a novel NeuRal Axiom Network (NeuRAN) framework that combines explicit structural and implicit axiom information without introducing additional ontologies. Specifically, the framework consists of a KG embedding module that preserves the semantics of triples and five axiom modules that encode five kinds of implicit axioms. These axioms correspond to five typical object property expression axioms defined in OWL2, including ObjectPropertyDomain, ObjectPropertyRange, DisjointObjectProperties, IrreflexiveObjectProperty and AsymmetricObjectProperty. The KG embedding module and axiom modules compute the scores that the triple conforms to the semantics and the corresponding axioms, respectively. Compared with KG embedding models and CKRL, our method achieves comparable performance on noise detection and triple classification and achieves significant performance on link prediction. Compared with TransE and TransH, our method improves the link prediction performance on the Hits@1 metric by 22.0% and 20.8% on WN18RR-10% dataset, respectively.

Keywords: Knowledge graph reasoning, knowledge graph embedding, noise detection, triple classification, link prediction

1. Introduction

Knowledge Graphs (KGs) are multi-relational directed graphs with entities and relations as nodes and edges. Typically, knowledge graphs contain a large number of triples in the form of (*subject entity*), relation, object entity),

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^a College of Computer Science and Technology, Zhejiang University, 38 Zheda Rd, Hangzhou, China

^b Department of Computer Science, University of Oxford, 15 Parks Rd, Oxford OX1 3QD, UK

^c School of Software Technology, Zhejiang University, 1689 Jiangnan Rd, Ningbo, China

^{*}Equal contribution.

^{**}Corresponding author. E-mail: zhang.wen@zju.edu.cn.

abbreviated as (s, r, o). Existing KGs like DBpedia [19], Freebase [1], Wikidata [30], and YAGO [13], have played a pivotal role in a broad range of applications, such as question answering [3] and recommender system [35]. Since KGs are usually automatically constructed, they may inevitably suffer from incompleteness and incorrectness. For example, 71% of people in Freebase have no place of birth, and 94% have no known parents [37]. While Wikipedia is estimated to have 2.8% of its statements wrong [23]. Thus many knowledge graph reasoning methods have been proposed and received increasing attention. There are two mainstream techniques, including symbolic- and embedding-based methods.

Symbolic-based methods [5,10,11,40] use predefined logic rules or ontologies for KG reasoning and can achieve good performance. For example, suppose the axiom *DisjointObjectProperties*(:hasParent :hasSpouse) that indicates the relations hasSpouse and hasParent are disjoint has already defined, then it is impossible for the two triples (Linda, hasSpouse, Bruce) and (Linda, hasParent, Bruce) to be correct at the same time. The reason is that a person's spouse can not be the parent of this person. Although such methods are more reliable and human-interpretable, they require rich ontologies that are usually missing or incomplete in KGs. Moreover, it is tedious to define and maintain axioms manually. Thus we explore how to encode implicit axioms with only triples for KG reasoning in this paper.

Embedding-based methods, such as translation-based methods [2,20,36], semantic-based methods [33,39] and neural network methods [6,25,26], embed entities and relations into low-dimensional vector space. They use vector computation to complete knowledge graphs, which is scalable and efficient. However, despite the success of embedding models, they mainly focus on structural information and neglect implicit axiom information. Take the implicit domain/range axiom as an example. For the correct triple (*Linda*, *hasSpouse*, *Bruce*), we can infer that it satisfies *domain/range* axiom without the type of the subject entity *Linda* and the object entity *Bruce*, and domain/range of the relation *hasSpouse*.

In this paper, we propose a neural axiom network framework NeuRAN for KG reasoning. This framework encodes explicit structural information through a knowledge graph embedding model and implicit axiom information through neural networks. The main idea is that although ontology information is not explicitly defined in the given KG, any correct triple satisfies all axioms. Thus, the score to measure the plausibility of each triple is composed of a score from structural information and five axiom scores from axiom information. Here we consider five different axioms corresponding to five typical object property expression axioms selected from OWL2 ontology language, l including ObjectPropertyDomain, ObjectPropertyRange, DisjointObjectProperties, IrreflexiveObjectProperty and AsymmetricObjectProperty. As domain and range axioms are related to type compatibility, we distinguish the type and semantic embeddings. Each entity has a type embedding and a semantic embedding. Each relation has two type embeddings (i.e., subject and object entity types excepted by the relation) and a semantic embedding. We encode the inherent structure of triples via an embedding module to learn semantic embeddings of entities and relations. In this paper, TransE and TransH are taken as examples of knowledge graph embedding modules to show the validity of our method. Any KGE model can be the KGE module. We introduce five axiom modules to encode axioms implicit in triples. The design of the axiom modules depends on the conditions that the axioms satisfy, as listed in Table 1. Specifically, for a triple (s, r, o), domain/range axiom module concentrates on type compatibility between subject/object entity type embedding expected by the relation and type embedding of the subject/object entity. Disjoint axiom module focuses on the compatibility of two relations with the same subject and object entity. Irreflexive axiom module encodes whether the relation is irreflexive and whether s = o. Meanwhile, asymmetric axiom module encodes whether the relation is asymmetric and whether (o, r, s) is also in the KG. For each axiom module, the output is a probability score ranging from 0 to 1, indicating how well the triple satisfies the axiom. The closer the value is to 1, the more likely the triple conforms to the axiom. For example in Fig. 1, the triple (*United Kingdom*, occupation, novelist) violates domain axiom. Therefore, the expected subject entity type embedding of the relation occupation and type embedding of the subject entity United Kingdom may get a low domain axiom score close to 0.

In summary, our main contributions are as follows:

- We raise the problem of neural axiom learning, in which axiom information is not given but can be reflected by and learned from existing triples in KGs.

¹https://www.w3.org/TR/owl2-primer/

Table 1

Five types of object property expression axioms selected from OWL2 ontology language. OP is the short for ObjectProperty. OPE denotes Object Property Expression, and x, y, z are entity variables. \triangle_I is a nonempty set called the object domain. $\overset{OP}{}$ is an object property interpretation function. When translating axioms into examples in KG according to condition, we replace OPE in axioms with a relation

Object Property Axioms	Condition	Examples
OPDomain(OPE CE)	$\forall (x, y) \in (OPE)^{OP} \text{ implies } x \in (CE)^C$	Domain(hasWife, Man)
OPRange(OPE CE)	$\forall (x, y) \in (OPE)^{OP} \text{ implies } y \in (CE)^C$	Range(hasWife, Woman)
$\overline{\text{DisjointOP}(\text{OPE}_1 \dots \text{OPE}_n)}$	$(\text{OPE}_j)^{\text{OP}} \cap (\text{OPE}_k)^{\text{OP}} = \emptyset$ for each $1 \leqslant j \leqslant n$ and each $1 \leqslant k \leqslant n$ such that $j \neq k$	Disjoint(hasParent, hasSpouse)
IrreflexiveOP(OPE)	$\forall x : x \in \Delta_I \text{ implies } (x, x) \notin (OPE)^{OP}$	Irreflexive(parentOf)
AsymmetricOP(OPE)	$\forall (x, y) \in (OPE)^{OP} \text{ implies } (y, x) \notin (OPE)^{OP}$	Asymmetric(hasChild)

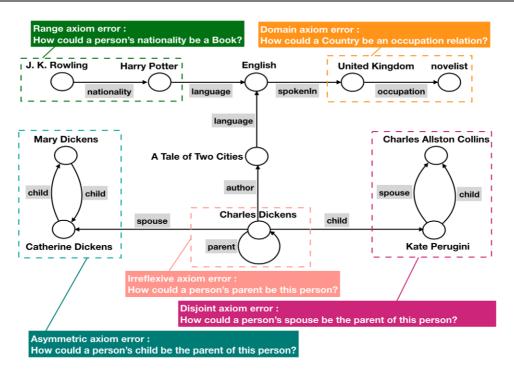


Fig. 1. In the hypothetical knowledge graph, there may exist erroneous triples. The reason for these errors is that the triples do not conform to the axioms considered in this paper, including *domain*, *range*, *disjoint*, *irreflexive* and *asymmetric* axioms.

- We propose a framework NeuRAN that uses a knowledge graph embedding module and five axiom modules to encode explicit structural and implicit axiom information, respectively.
- We evaluate NeuRAN on datasets with different ratios of noise. The experimental results demonstrate the effectiveness of our method on knowledge graph reasoning.

2. Related work

We discuss the following three lines of research work closely relevant to this paper, including symbolic-based reasoning, embedding-based reasoning and hybrid reasoning.

2.1. Symbolic-based reasoning

Symbolic-based reasoning methods aim at inferring new knowledge or detecting noises with the help of rules or ontologies and show good reasoning ability. For example, inductive logic programing (ILP) has been used to mine

logical rules and use the rules to learn a good predictor. However, it has limitations on the open-world assumption of KGs. AMIE [11] and AMIE+ [10] make up for this shortcoming by introducing an altered confidence metric based on the partial completeness assumption. With the rules generated with AMIE+, [14] proposes to discover inverse and symmetric axioms by applying the predefined reasoning rules. Due to the incompleteness of rules and axioms, and the time-consuming process of annotating them, existing methods using ontologies for reasoning are usually accompanied by the enrichment of ontology information. For example, the work [9] presents a set of inductive methods based on statistical inductive learning, consisting of correlation computing and association rule mining to enrich ontologies with disjointness axioms. It evaluates the validity of association rule mining by computing the precision and recall scores. Then [22] proposes an improvement of association rule mining for learning disjointness axioms and applies the learned axioms to inconsistency detection. In addition to disjoint axioms, enriching DBpedia ontology with domain and range restrictions and class disjointness axioms is also discussed [31]. The enhanced ontologies are further used for error detection.

2.2. Embedding-based reasoning

Knowledge graph embedding methods embed entities and relations of a KG into a continuous vector space to preserve the structure information of the KG. There are three categories of embedding models: translational distance, semantic matching and neural network models. Translational distance models learn embeddings by translating a subject entity to an object entity through a relation. For example, TransE [2] represents entities and relations in the same vector space and assumes (s + r) to be close to o, where s, r, o are vector embeddings for s, r and o respectively. However, it has difficulty dealing with complex relations. To overcome the flaws, TransH [36] introduces relation-specific hyperplanes to allow entities to have different embeddings in different relations. TransR [20] builds entity and relation embeddings in separate entity and relation spaces. TransD [16] constructs mapping matrices dynamically. Similarly, TorusE [8] and RotatE [29] use lie groups and rotations for translation, respectively. Semantic matching models measure plausibility by matching the implicit semantics of entities and relations. DistMult [39] uses a bilinear model to represent entities and relations. ComplEx [33] extends DistMult by introducing complexvalued embeddings to better model asymmetric relations. HolE [27] uses the circular correlation of embeddings to learn compositional representations and semantically matches circular correlation with the relation embedding. Moreover, researchers have raised interest in applying neural networks for knowledge graph reasoning. ConvE [6] and ConvKB [25] employ convolutional neural networks to achieve better link prediction performance. CapsE [26] explores a capsule network to model triples. KGTtm [17] and CKRL [38] measure the trustworthiness or confidence of triples.

2.3. Hybrid reasoning

There is also a line of work concerning hybrid methods for KG reasoning, such as the combination of symbolic and embedding-based reasoning, and the combination of symbolic and statistical reasoning. For the former methods, TransC [21] learns the SubClassOf axiom between types by encoding each type as a sphere and each entity as a vector. Besides, SetE [42] computes the two axioms SubClassOf and SubPropertyOf in subsumption by employing linear programming methods on embeddings, focusing on domain, range or subClassOf axioms. Recently, IterE [41] iteratively learns embeddings and rules, and considers seven object property expression axioms for rule learning. It combines rule learning and embedding learning to improve the quality of sparse entity embeddings by injecting new triples about sparse entities according to the scores of the axioms. As for the latter, the statistic-based methods, such as SDType and SDValidate [28], exploit statistical distributions of types and relations. SDType deduces missing type information based on the statistical distribution of types in the subject or object position of the relation. While SDValidate measures the deviation between actual types of the subject/object entity and the apriori probabilities given by the distribution. Furthermore, [4] first exploits a combination of entailment vectors, entailment weights, and a consistency vector to encode knowledge as embeddings in ontology streams to deal with concept drifts. It takes the concepts as input. The difference is that we design the axiom modules with the help of the definition of axioms.

3. Method

We begin this section by briefly describing some notations. We denote a knowledge graph as $\mathcal{G} = \{(s, r, o) \subset \mathcal{E} \times \mathcal{R} \times \mathcal{E}\}$, where $s, o \in \mathcal{E}$, $r \in \mathcal{R}$, \mathcal{E} is the entity set, and \mathcal{R} is the relation set. (s, r, o) is a triple indicating the relation r between the subject entity s and the object entity s. Throughout this paper, we use bold letters to denote vectors. For example, s, r, s are the embedding vectors of s, s, s. The abbreviations DM (dm), RG (rg), DIS (dis), IRR (irr) and ASY (asy) respectively correspond to the implicit *domain*, range, disjoint, irreflexive and asymmetric axioms.

Then, we introduce the neural axiom network NeuRAN which combines a knowledge graph embedding module and five axiom modules (Section 3.1). Afterward, we introduce the KGE module that encodes explicit structural information (Section 3.2) and the five axiom modules that aim to encode five kinds of implicit axiom information (Section 3.3).

3.1. Neural axiom network

We present our neural axiom network NeuRAN in Fig. 2, where the overall score of each triple is composed of a semantic score from the KGE module and five axiom scores from five axiom modules (i.e., *domain*, *range*, *disjoint*, *irreflexive* and *asymmetric* axiom modules). The score of each axiom module indicates the probability that the axiom holds. The assumption is that the probability values of these axioms intensify or mitigate the probability

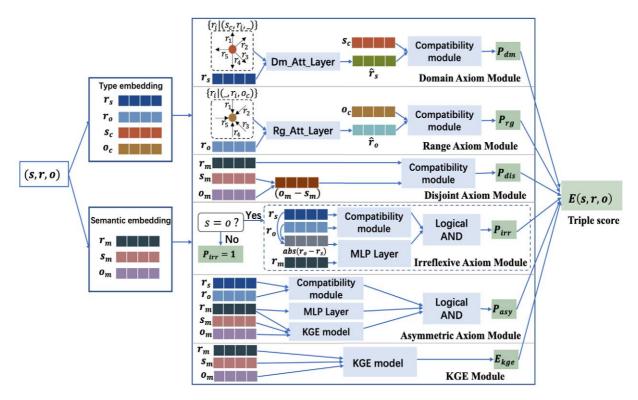


Fig. 2. The key idea of our framework. For the input triple (s, r, o), we use a type embedding (s_c, o_c) and a semantic embedding (s_m, o_m) to represent the entities, and use two type embeddings (r_s, r_o) and a semantic embedding (r_m) to represent the relation. The triple score is composed of the scores from the six modules. The domain/range axiom module calculates the compatibility between the subject/object entity type embedding and the relation embedding generated via a domain/range attention layer. The disjoint axiom module calculates the compatibility between the semantic embedding of the input relation and other relations with the same subject and object entities. The irreflexive and asymmetric axiom modules calculate the axiom scores using the type and semantic embeddings of the entities and relations. The KGE module is a knowledge graph embedding model.

of the existence of a triple. Thus, the score of the triple (s, r, o) is defined as:

$$E(s, r, o) = E_{\text{kge}} + \lambda \cdot \left[(1 - P_{\text{dm}}) + (1 - P_{\text{rg}}) + (1 - P_{\text{dis}}) + (1 - P_{\text{irr}}) + (1 - P_{\text{asy}}) \right]$$
(1)

The energy function E(s,r,o) consists of the score $E_{\rm kge}$ from the knowledge graph module and five axiom scores from the axiom modules. λ is the weight of axiom scores. $E_{\rm kge}$ is to compute a structure-based score, which can be obtained via any knowledge graph embedding models [34]. We use TransE and TransH as examples. A lower $E_{\rm kge}$ indicates that the triple is more likely to be correct. The axiom scores $P_{\rm dm}$, $P_{\rm rg}$, $P_{\rm dis}$, $P_{\rm irr}$ and $P_{\rm asy}$ correspond to probabilities that the corresponding axioms are satisfied, where dm, rg, dis, irr and asy are respectively domain, range, disjoint, irreflexive and asymmetric axioms. Therefore, the higher $P_{\rm dm}$, $P_{\rm rg}$, $P_{\rm dis}$, $P_{\rm irr}$, $P_{\rm asy}$, and the lower $(1-P_{\rm dm})$, $(1-P_{\rm rg})$, $(1-P_{\rm dis})$, $(1-P_{\rm irr})$, $(1-P_{\rm asy})$ imply that the triple satisfies the corresponding neural axiom with a higher probability.

Following the conventional training strategy of previous models, we train NeuRAN based on the local-closed world assumption. In this case, the observed triples in KGs are regarded as positive triples, while the unobserved ones are regarded as negative triples. We utilize a margin-based ranking loss on pair-wise score functions (i.e., E(s, r, o) and E(s', r', o')) for training, the loss function \mathcal{L} is defined as:

$$\mathcal{L} = \sum_{(s,r,o)\in T} \sum_{(s',r',o')\in T'} \max(0, E(s,r,o) + \gamma - E(s',r',o'))$$

$$\tag{2}$$

where γ is a margin hyper-parameter, E(s, r, o) and E(s', r', o') are respectively the overall energy function of the positive triple (s, r, o) and the negative triple (s', r', o'). T and T' are the positive and negative triple sets. As negative triples and axioms are not given, we generate negative triples by randomly corrupting the subject or object entity and make sure the replaced triples do not exist in the knowledge graph:

$$T' = \left\{ \left(s', r, o \right) | s' \in \mathcal{E} \right\} \cup \left\{ \left(s, r, o' \right) | o' \in \mathcal{E} \right\}, (s, r, o) \in T, \left(s', r, o \right) \notin T \text{ and } \left(s, r, o' \right) \notin T$$
 (3)

The training objective is to minimize the loss function \mathcal{L} to learn embeddings of entities and relations and parameters involved in axiom modules. The learned embeddings and parameters are applied to complete downstream tasks, such as noise detection, triple classification and link prediction.

It is worth mentioning that, we attempt to introduce type embeddings in the design of the model. Considering domain/range axioms are associated with type compatibility, and type information is not provided, we distinguish type embeddings from semantic embeddings. Following the type-sensitive models TypeDM and TypeComplex [15], each entity is represented as two vectors (a type embedding and a semantic embedding), and each relation is represented as three vectors (two type embeddings and a semantic embedding). Take the triple (s, r, o) as an example. For entities, we use type embeddings $(s_c$ and $o_c)$ and semantic embeddings $(s_m$ and $o_m)$ to represent the subject entity s and the object entity s. For the relation, r_s and r_o represent subject type and object type embeddings expected by the relation r, and r_m is the semantic embedding of r.

3.2. KG embedding module

The knowledge graph embedding module of the framework concerns the learning of a function $E_{\rm kge}$, which is designed to score each triple based on the structural information in KGs. Our framework can use any knowledge graph embedding model as the knowledge graph embedding module. In the experiments, we take the two embedding models TransE and TransH as examples to verify our method.

3.2.1. TransE

TransE is the simplest translation-based model, which interprets relations as translating operations between subject and object entities. Given a triple (s, r, o), it follows the assumption that $s + r \approx o$ when (s, r, o) holds. Thus, the semantic score of the triple based on TransE is calculated as:

$$E_{\text{kge}} = \|s_m + r_m - o_m\|_{L_1/L_2} \tag{4}$$

where L_1 and L_2 respectively denote the L_1 and L_2 norm. s_m , r_m and o_m are the semantic embeddings of the subject entity, the relation and the object entity, respectively. The smaller value of the scoring function E_{kge} , the higher the probability that the triple is correct.

3.2.2. TransH

TransH extends TransE by translating on hyperplanes, which models the relation r as a vector on a hyperplane with w_r as the normal vector. It enables an entity to have distinct representations when involved in different relations. Similar to TransE, the score function of TransH is defined as:

$$E_{\text{kge}} = \|(s_m)_{\perp} + r_m - (o_m)_{\perp}\|_{L_1/L_2}$$
(5)

where the projections $(s_m)_{\perp} = s_m - w_r^{\top} s_m w_r$, and $(o_m)_{\perp} = o_m - w_r^{\top} o_m w_r$. It restricts $||w_r||_2 = 1$. The score is low if (s, r, o) holds and is high otherwise.

3.3. Five axiom modules

In addition to focusing on structural information, we consider the inherent implicit axioms in triples. Although axioms are not pre-given, it is intuitive that a correct triple is also a logically consistent triple. Any correct triple satisfies all the five axioms, including *domain*, *range*, *disjoint*, *irreflexive*, and *asymmetric* axioms. For example, in the case of missing domain and range of the relation *nationality* and types of the entities *J. K. Rowling* and *United Kingdom*, we can infer the triple (*J. K. Rowling*, *nationality*, *United Kingdom*) satisfies *domain* and *range* axioms by its correctness.

The design of the axiom modules relies on the definition of these axioms. To be specific, for *domain/range* axioms, we use the type embedding of the subject/object entity expected by the relation r_s/r_o and the type embedding of the subject/object entity s_c/o_c to calculate a type compatibility score. For *disjoint* axiom, we explore the semantic compatibility of any two relations with the same subject and object entities. We assume that $(o_m - s_m)$ represents the shared semantic embedding of the relation for the subject to be s and object to be s. Then the similar score of r_m and $(o_m - s_m)$ will be calculated to reflect how well the disjoint axiom is satisfied. For *irreflexive* axiom, whether the relation is irreflexive and whether the subject entity is the same as the object entity (s = o?) are considered. For *asymmetric* axiom, whether the relation is asymmetric and whether the symmetric triple of the input triple exists $((o, r, s) \in G?)$ are concerned. We then introduce these typical axioms in detail.

3.3.1. Domain axiom module

Domain axiom module focuses on type compatibility between the subject entity type expected by the relation r and the type of the subject entity s. TypeDM uses the function $C(s_c, r_s) = \sigma(s_c \cdot r_s)$ to measure the compatibility by calculating a score with the type embedding of subject entity s_c and the subject entity type embedding expected by the relation r_s . However, the subject type expected by the given relation may be diverse. For example, given the triple (Soul(film), language, English), the subject type expected by the relation language can be an entity in the class of Person, Book or Film. We consider both the current relation and the other relations of the subject entity to precisely capture the type of the subject entity expected by the relation. Suppose the subject entity has relations starring and running time, we can infer that the subject entity expected by the relation may be in the class of Film. As the relations may have correlations with the given relation, such as starring and language, or differ greatly such as running time and language, they contribute differently to the subject entity type embedding expected by the currently given relation. We apply an attention mechanism to the relation r and the relation set of the subject entity $\mathcal{R}(s) = \{r_i | (s, r_i, e) \in \mathcal{G}\}$, where e denotes any entity in the KG. By adopting a domain attention layer (Dm_Att_Layer), we generate the subject type embedding expected by the relation \hat{r}_s based on the relations in $\mathcal{R}(s)$. We compute an attention weight for each relation of the subject entity, and the importance is denoted by a_i . It reflects how relevant or important the relation r_i is to r_s .

$$a_i = f(\mathbf{r}_s, \mathbf{r}_i) = \mathbf{r}_s^T \mathbf{r}_i, \quad r_i \in \mathcal{R}(s)$$
 (6)

We apply *softmax* over a_i to get the relative attention values.

$$p_i = \frac{\exp(a_i)}{\sum_{r_j \in \mathcal{R}(s)} \exp(a_j)}$$
 (7)

where j denotes the jth relation of the subject entity. The new embedding of the subject entity type expected by the relation $\hat{r_s}$ is the sum of the product of the representation of each relation and the relation weighted by attention values of the considered relation.

$$\hat{\mathbf{r}}_s = \sum_{r_i \in \mathcal{R}(s)} p_i r_i \tag{8}$$

Then the type compatibility is calculated via a compatibility module, and the likelihood of *s* and *r* satisfying *domain* axiom can be defined as follows:

$$P_{\rm dm} = f(\mathbf{s_c}, \mathbf{r_s}) = \sigma(\mathbf{s_c} \cdot \hat{\mathbf{r_s}}) \tag{9}$$

where σ denotes the sigmoid function.

3.3.2. Range axiom module

Range axiom module focuses on type compatibility between the object entity type expected by the relation r and the type of the object entity o. Similarly, TypeDM uses $C(o_c, r_o) = \sigma(o_c \cdot r_o)$ to compute the compatibility score between the type embedding of the object entity o_c and the object entity type embedding expected by the relation r_o , where the score indicates the satisfaction of range axiom. However, a relation can have object entities with very different types. For example, the object entity of the relation hasPart can be Leg in (Table, hasPart, Leg), or NewYorkBay in (Atlantics, hasPart, NewYorkBay). Similar to the issue in domain axiom, object entities expected by a relation may exhibit diverse roles within the same relation. The other relations connected to the object entity make different contributions to the object entity's type embedding expected by the relation. We apply a range attention layer (Rg_Att_Layer) to the relations connected to the object entity to more accurately discern the expected object entity type associated with the given relation. The relation set that connected to the object entity o is denoted as $\mathcal{R}(o) = \{r_i | (e, r_i, o) \in \mathcal{G}\}$. We generate the object entity type embedding expected by the relation $\hat{r_o}$ based on all the relations in $\mathcal{R}(o)$. The importance of each relation to r denoted by r is calculated as:

$$b_i = f(\mathbf{r_o}, \mathbf{r_i}) = \mathbf{r_o}^T \mathbf{r_i}, \quad r_i \in \mathcal{R}(o)$$
(10)

We then apply *softmax* over b_i to get the relative attention values.

$$q_i = \frac{\exp(b_i)}{\sum_{r_k \in \mathcal{R}(o)} \exp(b_k)}$$
 (11)

where k denotes the kth relation in the connected relations of the object entity. The generated embedding $\hat{r_o}$ is the sum of the product of each relation connected to o and the relation weighted by attention values of the considered relation r.

$$\hat{\mathbf{r_o}} = \sum_{r_i \in \mathcal{R}(o)} q_i r_i \tag{12}$$

The compatibility probability whether the triple satisfies *range* axiom is calculated by a compatibility module and is defined as:

$$P_{\rm rg} = f(\boldsymbol{o_c}, \boldsymbol{r_o}) = \sigma(\boldsymbol{o_c} \cdot \hat{\boldsymbol{r_o}}) \tag{13}$$

where σ denotes the sigmoid function.

3.3.3. Disjoint axiom module

Disjoint axiom module focuses on the compatibility of the semantic embeddings of two relations with the same subject and object entities. For example, given the correct triple (*John*, *spouse*, *Mary*), and other two triples (*John*, *friend*, *Mary*) and (*John*, *child*, *Mary*), the disjoint axiom module computes probability scores of the two relation pairs including (*spouse*, *friend*), and (*spouse*, *child*). Then we can infer (*John*, *friend*, *Mary*) is a correct triple, and (*John*, *child*, *Mary*) is an incorrect triple. The reason is that the disjoint probability score of *spouse* and *friend* is high as they can exist between two persons simultaneously. In contrast, the score of *spouse* and *child* is low as a person's spouse can not be that person's child. In other words, *spouse* and *child* are defined to be semantically *disjoint*. Following the condition of *disjoint* axiom, we have to traverse the whole knowledge graph to find all the relations with *s* being the subject entity and *o* being the object entity. The relation set is $\mathcal{R}(s,o) = \{r_k | (s,r_k,o) \in \mathcal{G}, r_k \neq r\}$. However, calculating the semantic compatibility of the relation pairs (r,r_k) is time-consuming. We copy the idea from TransE for simplicity, which holds the view that $s+r \approx o$ to reduce time cost. Specifically, we regard $(o_m - s_m)$ as the unified representation of relations in triples with *s* and *o* being the subject and object entity. Therefore, the semantic judgment of this axiom can be simplified to calculate the compatibility score of $(o_m - s_m)$ and r_m , which is defined as:

$$P_{\text{dis}} = f(\mathbf{r}_m, (\mathbf{o}_m - \mathbf{s}_m)) = \sigma(\mathbf{r}_m \cdot (\mathbf{o}_m - \mathbf{s}_m))$$
(14)

where σ denotes the sigmoid function.

3.3.4. Irreflexive axiom module

Irreflexive axiom module considers two aspects of judgment. One is the property of the relation (*i.e.*, whether r is irreflexive), and the other is whether the subject and object entity are equal (*i.e.*, whether s and o are the same entity). In OWL2, a relation is irreflexive means that no entity can be related to itself by such a relation. Thus, only the two conditions the relation r is irreflexive and s = o are fulfilled simultaneously, the triple violates irreflexive axioms. For example, for the irreflexive relation hasParent, it is intuitively that (John, hasParent, John) is an incorrect triple.

Due to the judgment of s=o can be conducted directly without the need to represent the two entities as vectors, we take it as the first step. If s=o, we further consider the property of the relation. Otherwise, the probability that the triple conforms to *irreflexive* axiom is equal to 1 as $s\neq o$ already violates one of the two conditions. For the case of s=o, we can infer that types of s and o are the same ($s_c=o_c$). Regarding the property of the relation, we expect types of the subject entity r_s and the object entity expected by the relation r_o to be compatible with s and s, respectively. That is s, and s, and s, and s, are compatible to measure the type constraint, which is calculated as s, and s, we use a compatibility module to measure the type constraint, which is calculated as s, and s, we utilize a multilayer perceptron (MLP) layer to encode the relation's semantics, domain and range. The probability that a triple satisfies s irreflexive axiom is calculated through the Logic AND operation and is defined as:

$$P_{\text{irr}} = \begin{cases} 1, & \text{if } s \neq o \\ \sigma(W_1[\mathbf{r_m}; g(\mathbf{r_s}, \mathbf{r_o})]) * \sigma(\mathbf{r_o} \cdot \mathbf{r_s}), & s = o \end{cases}$$
 (15)

where g(x, y) is a function, and g(x, y) = abs(x - y). $W_1 \in \mathbb{R}^{1 \times (d_m + t_m)}$, and d_m are the dimension of the semantic and type embedding, respectively. σ denotes the sigmoid function. [;] denotes the concatenation operation.

3.3.5. Asymmetric axiom module

Asymmetric axiom module considers two aspects of judgment as well, which are the property of the relation (i.e., whether r is asymmetric) and the existence of the symmetric triple of the given triple (i.e., whether (s, r, o) and (o, r, s) are both correct in the same KG). In OWL2, a relation is asymmetric means that if it connects s with s, it never connects s with s. In other words, for the correct triple (s, r, o), if s is an asymmetric relation and s appears in the same s as s as s is incorrect for the violation of asymmetric axiom. For example, given the correct triple s is incorrect for that s is incorrect for the s asymmetric axiom as s asymmetric axiom as s asymmetric.

In this axiom, we begin with determining the property of the relation by focusing on the semantic embedding r_m . We take a multi-layer perceptron (MLP) layer to capture the semantics of the relation. Secondly, we consider the compatibility of r_s and r_o as a condition of the property of the relation. The reason is that, if r is symmetric, we can infer $r_s \approx r_o$ from the observations that $r_s \approx s_c$, $r_o \approx o_c$ from the triple (s, r, o), and $r_s \approx o_c$, $r_o \approx s_c$ from the triple (o, r, s). Thirdly, we use the simplest knowledge graph embedding model TransE to check whether (o, r, s) exists. Since the above conditions together determine whether a triple violates this axiom, we introduce a Logical AND operation as well. Therefore, the asymmetric axiom network is defined as follows:

$$f_{\text{kge}} = \sigma(o_m + r_m - s_m) \tag{16}$$

$$P_{\text{asy}} = \sigma(W_2(\mathbf{r_m})) * \sigma(\mathbf{r_o} \cdot \mathbf{r_s}) * f_{\text{kge}}$$
(17)

where $W_2 \in \mathbb{R}^{1 \times d_m}$, and σ denotes the sigmoid function.

4. Experiments

We evaluate our proposed method NeuRAN on three main knowledge graph reasoning tasks: noise detection, link prediction, and triple classification. Our code is available at https://github.com/JuanLi1621/NeuRAN.

4.1. Experimental settings

Datasets. In this paper, we use two popular benchmark datasets: FB15K237 [32] and WN18RR [6] to evaluate NeuRAN. They are constructed from FB15K and WN18 by removing inverse relations to solve test leakage. FB15K is a relatively dense subset extracted from the collaborative knowledge graph Freebase [1], which consists of billions of real-world facts. WN18 is a subset of WordNet [24] that describes relations between words.

Error Imputation. Since KGs are constructed in an automated or semi-automated way, noises can not be avoided. However, existing knowledge graph reasoning methods assume that triples in KGs are positive triples. Thus there are no pre-given noisy triples in FB15K237 and WN18RR. In order to verify our method, we generate new datasets with different noise rates based on the two datasets to simulate the real noisy knowledge graphs. Before generating noises, for each dataset with training, validation and test sets, we generate negative triples for the validation and test sets. The positive and negative triples in the validation set are used to find the optimum thresholds for each relation. To evaluate the performance of NeuRAN on triple classification, the positive and negative triples in the test set are classified as positive or negative triples based on both the triple scores and the thresholds. Here, we directly use the negative triples generated in OpenKE.² Then, we randomly sample positive triples from the training set with different noise rates and generate the same number of negative triples as the sampled triples. Specifically, we corrupt either the subject or object entity of a triple with equal probability and ensure the generated negative triples do not exist in the KG. The generated negative triples are regarded as noises. All three tasks are evaluated on these simulated noisy datasets. For each dataset, we construct three noisy datasets with the ratio of negative triples to be 10%, 20%, and 40% of the positive triples. The generated negative triples (noises) with different ratios listed in Table 3 will be added to the training set as part of the training triples and labeled as positive triples. For example, for the datasets FB15K237-10%, FB15K237-20% and FB15K237-40%, the number of triples in the training set is 299326 (272115 + 27211), 326538 (272115 + 54423) and 380961 (272115 + 108846), respectively. The number of positive triples in the validation and test sets is 17535 and 20466, which is the same as FB15K237. Besides, the number of negative triples in the validation and test sets is the same as the number of positive triples. All the three noisy datasets share the same entities and relations with the original dataset. The detailed statistics of the two datasets and the generated noisy datasets are shown in Table 2 and 3.

Baselines. We choose TransE or TransH as the knowledge graph embedding module and compare our methods (i.e., NeuRAN(TransE), NeuRAN(TransH)) with them. Results of TransE and TransH are produced by running

²https://github.com/thunlp/OpenKE/tree/OpenKE-Tensorflow1.0/benchmarks

Table 2 Statistics of FB15K237 and WN18RR

Dataset	#Ent	#Rel	#Train	#Valid	#Test
FB15K237	14541	237	272115	17535	20466
WN18RR	40943	11	86835	3034	3134

Table 3
Statistics of negative triples generated from FB15K237 and WN18RR

Datasets	FB15K237-10%	FB15K237-20%	FB15K237-40%
#Neg triple	27211	54423	108846
Datasets	WN18RR-10%	WN18RR-20%	WN18RR-40%
#Neg triple	8683	17367	34734

Table 4

Noise detection results on noisy datasets with different ratios based on FB15K237 and WN18RR. The numbers are auc values

	FB15K237-10%	FB15K237-20%	FB15K237-40%	WN18RR-10%	WN18RR-20%	WN18RR-40%
TransE	0.9805	0.9799	0.9801	0.9370	0.9305	0.9018
CKRL(TransE)	0.9809	0.9804	0.9653	0.9337	0.9255	0.8971
NeuRAN(TransE)	0.9807	0.9807	0.9802	0.9403	0.9337	0.9141
TransH	0.9763	0.9746	0.9758	0.9331	0.9169	0.8614
CKRL(TransH)	0.9683	0.9697	0.9663	0.9279	0.9091	0.8527
NeuRAN(TransH)	0.9781	0.9783	0.9796	0.9340	0.9239	0.8780

OpenKE [12]. We also consider CKRL(TransE) and CKRL(TransH) as baselines, which introduce path information for knowledge graph reasoning in noisy KGs. Results of CKRL(TransE) and CKRL(TransH) are reproduced by us. In the following tasks, the results of TransE, TransH, CKRL(TransE) and CKRL(TransH) are all obtained in this way.

Training Details. We use SGD [7] or Adam [18] to optimize the model for different tasks on different datasets. We select the learning rate from $\{0.01, 0.1, 0.5, 1\}$, the margin among $\{2,4,6,8,10\}$, the batch size from $\{100, 500\}$, dimension of the type from $\{20, 50, 100, 200\}$, dimension of the semantic from $\{50, 100, 200, 300\}$, the combination weight of the axiom scores λ from $\{0.01, 0.05, 0.1, 0.5, 1\}$. The number of training epochs is set as 1000.

4.2. Noise detection

To verify the capability of our method on noise detection task, we follow the setting of KG noise detection proposed in [38]. It aims to detect possible noises in noisy KGs according to the scores of triples and can be viewed as triple classification task on the training set.

Evaluation Protocol. First of all, we compute the score of the triple (s, r, o) via the energy function $E(s, r, o) = E_{\text{kge}} + \lambda \cdot [(1 - P_{\text{dm}}) + (1 - P_{\text{rg}}) + (1 - P_{\text{dis}}) + (1 - P_{\text{irr}}) + (1 - P_{\text{asy}})]$. Then all triples in the training set will be ranked based on the scores. The lower the triple score, the more valid the triple is. Triples with higher values of the energy function tend to be noises. We consider the evaluation indicator the Area Under the ROC Curve (*auc value*) to examine how well the method classifies the noises as errors. Before calculating the AUC metric, we normalize the energy function scores into the [0, 1] interval. Values close to 0 indicate correct triple, and values close to 1 indicate incorrect triples.

Result Analysis. Evaluation results on noisy datasets generated based on FB15K237 and WN18RR can be found in Table 4. We observe that: (1) Regardless of whether the embedding module is TransE or TransH, our models achieve comparable performance or slightly outperform TransE, CKRL(TransE), TransH, and CKRL(TransH) on the two datasets WN18RR and FB15K237 with different noise rates (i.e., WN18RR-10%, WN18RR-20%,

WN18RR-40%, FB15K237-10%, FB15K237-20%, and FB15K237-40%). (2) When the complex relations are well encoded, for example, in TransH. Our model with axiom information performs better than path information on noise detection on WN18RR- and FB15K237-based datasets. (3) With the increase of noises, the ability of baselines and our models to detect noises decreases on WN18RR-based datasets. However, it may increase on FB15K237-based datasets, which indicates that the more relations and triples in noisy datasets, the more valid information may be introduced, even though these triples may be noises.

We can thus conclude that implicit axiom information is helpful for noise detection and is better reflected on datasets with a large number of relations and triples.

4.3. Triple classification

Triple classification aims to judge whether a triple in the test set is correct or not, according to triple scores calculated by the energy function $E(s, r, o) = E_{\text{kge}} + \lambda \cdot [(1 - P_{\text{dm}}) + (1 - P_{\text{rg}}) + (1 - P_{\text{dis}}) + (1 - P_{\text{irr}}) + (1 - P_{\text{asy}})]$, which can be viewed as a binary classification task on the test set.

Evaluation Protocol. As the test sets of the datasets used for triple classification only have correct triples, we generate negative triples by randomly corrupting the subject or object entity of correct triples. For the validation and test sets, the number of negative triples is the same as the number of positive triples. Thus there are labeled positive and negative triples in the two sets. For example, for WN18RR-based datasets, the number of triples is 6068 in the validation set and 6268 in the test set. As for triple classification, we learn a relation-specific threshold δ_r for every relation. δ_r is optimized by maximizing classification accuracies on the validation set. Given a triple (s, r, o), if the score obtained by the energy function is below δ_r , it is classified as positive, otherwise negative. We use accuracy(ACC), precision(P) and recall(R) as the evaluation metrics.

Result Analysis. Table 5 and 6 show the detailed evaluation results of triple classification. From the two tables, we can observe that: (1) Regarding the three metrics, our method outperforms baselines on the WN18RR-based datasets and achieves the best results. It confirms that learning knowledge representations with axiom information can help triple classification. (2) On the FB15K237-based dataset, the results are comparable with baselines.

Table 5

Triple classification results on WN18RR, WN18RR-10%, WN18RR-20% and WN18RR-40%. "ACC", "P" and "R" are the abbreviation of "accuracy", "precision" and "recall", respectively

Methods	,	WN18RR-10%			WN18RR-20%			WN18RR-40%		
	ACC	P	R	ACC	P	R	ACC	P	R	
TransE	0.8764	0.9232	0.8210	0.8575	0.8889	0.8172	0.8355	0.9046	0.7502	
CKRL(TransE)	0.8759	0.9201	0.8232	0.8574	0.8994	0.8047	0.8350	0.9127	0.7409	
NeuRAN(TransE)	0.8856	0.9281	0.8360	0.8703	0.9100	0.8197	0.8598	0.9328	0.7754	
TransH	0.8618	0.9216	0.7910	0.8444	0.9039	0.7709	0.8146	0.8772	0.7317	
CKRL(TransH)	0.8556	0.9233	0.7757	0.8403	0.8829	0.7846	0.8116	0.8629	0.7409	
NeuRAN(TransH)	0.8687	0.9300	0.7974	0.8598	0.9040	0.8050	0.8323	0.8802	0.7693	

Table 6
Triple classification results for FB15K237-10%, FB15K237-20% and FB15K237-40%. "ACC", "P" and "R" are the abbreviation of "accuracy", "precision" and "recall", respectively

Methods	FB15K237-10%			F	FB15K237-20%			FB15K237-40%		
	ACC	P	R	ACC	P	R	ACC	P	R	
TransE	0.7758	0.7743	0.7786	0.7605	0.7353	0.8140	0.7422	0.7269	0.7759	
CKRL(TransE)	0.7767	0.7728	0.7839	0.7579	0.7407	0.7936	0.7420	0.7314	0.7651	
NeuRAN(TransE)	0.7810	0.7846	0.7749	0.7656	0.7711	0.7554	0.7484	0.7497	0.7459	
TransH	0.7978	0.8023	0.7904	0.7831	0.7816	0.7857	0.7623	0.7754	0.7387	
CKRL(TransH)	0.7835	0.7922	0.7686	0.7660	0.7669	0.7642	0.7473	0.7528	0.7365	
NeuRAN(TransH)	0.7882	0.8080	0.7561	0.7784	0.7891	0.7600	0.7617	0.7796	0.7299	

The improvements on WN18RR-10%, WN18RR-20% and WN18RR-40% are more evident than on FB15K237-10%, FB15K237-20% and FB15K237-40%. It demonstrates that implicit axiom information is more effective on a dataset with a smaller number of relations and triples. (3) Compared with TransE, TransH, CKRL(TransE) and CKRL(TransH), the higher the noise rate, the smaller the decrease in the accuracy metric of our method on WN18RR-10%, WN18RR-20% and WN18RR-40%. It indicates that on noisy datasets, triple classification results of NeuRAN can be more robust than baselines on small datasets.

From the triple classification results, we can conclude that the combination of implicit axiom and structural information reflected by existing triples in knowledge graphs works better than using only structural information on datasets with a small number of relations and triples. In comparison, path information is more helpful when the number of relations and triples is large.

4.4. Link prediction

To show that axiom information could improve the embedding learning of entities and relations and further help complete knowledge graphs, we conduct link prediction to evaluate the performance of knowledge graph completion. This task aims to predict the missing entity when given one entity and one relation of a triple, including subject entity prediction (?, r, o) and object entity prediction (s, r, ?).

Evaluation Protocol. For each test triple, suppose the subject entity prediction (?, r, o) with the correct subject entity s. We first take all entities $e \in \mathcal{E}$ in the dataset as candidate predictions, and then replace the missing part with each entity e and calculate scores for the triples in $\mathcal{T} = \{(e, r, o) | e \in \mathcal{G}\}$. Subsequently, we rank these scores in ascending order, and the rank of the correct entity is stored. The object entity prediction is in the same way. The evaluation metrics are MRR and Hits@N, where MRR is the mean reciprocal rank of the ranks of all test triples, and Hits@N (N = 1, 3) is the proportion of ranks within e0 of all the test triples. A higher MRR and a higher Hits@1, 3 should be achieved by a good embedding model. We call this 'raw' setting. If we filter out the corrupted triples that exist in the training, validation or test set before ranking, the evaluation setting is called 'filter'. In this paper, we report the evaluation results of the filter setting.

Result Analysis. Link prediction results are shown in Table 7 and 8. We analyze the results as follows: (1) The link prediction results of our method are improved compared with baselines on WN18RR-10%, WN18RR-20% and WN18RR-40% datasets, as well as on FB15K237-10%, FB15K237-20% and FB15K237-40%. It confirms that the learned knowledge graph embeddings' quality is better and could help complete KGs. Besides, it indicates axiom information can be more useful than path information on noisy datasets. (2) On WN18RR-10%, WN18RR-20% and WN18RR-40% datasets, our method achieves the best performance on all metrics. The improvements are significant on all metrics, especially on Hits@1. It demonstrates that axiom information is of great help in improving the predictive ability of a missing triple when the dataset has fewer relations and triples. (3) On FB15K237-10%, FB15K237-20% and FB15K237-40%, although the improvements of the results are less prominent compared with WN18RR-based datasets, the results are better than baselines. It reaffirms that our method can improve link prediction, and the more relations and triples, the more information and noises brought by axiom information. Therefore, the advantages of implicit axiom information would not be as significant as in small-scale datasets.

Table 7
Link prediction results on FB15K237-10%, FB15K237-20% and FB15K237-40%

	FB15K237-10%			FB15K237-20%			FB15K237-40%		
	MRR	Hit@		MRR	Hit@		MRR	Hit@	
		3	1		3	1		3	1
TransE	0.258	0.299	0.159	0.240	0.279	0.144	0.230	0.270	0.137
CKRL(TransE)	0.252	0.294	0.150	0.236	0.278	0.136	0.225	0.268	0.129
NeuRAN(TransE)	0.284	0.313	0.199	0.269	0.292	0.189	0.251	0.273	0.176
TransH	0.241	0.296	0.125	0.213	0.270	0.094	0.193	0.248	0.078
CKRL(TransH)	0.194	0.254	0.070	0.172	0.229	0.050	0.156	0.209	0.041
NeuRAN(TransH)	0.288	0.317	0.203	0.270	0.293	0.189	0.249	0.272	0.173

Table 8	
Link prediction results on WN18RR-10%, WN18RR-20% and WN18RR-40%)

	WN18RR-10%			WN18RR-20%			WN18RR-40%		
	MRR	Hit@		MRR	Hit@		MRR	Hit@	
		3	1		3	1		3	1
TransE	0.211	0.351	0.036	0.206	0.349	0.031	0.193	0.334	0.027
CKRL(TransE)	0.215	0.349	0.044	0.205	0.340	0.034	0.154	0.233	0.024
NeuRAN(TransE)	0.342	0.393	0.256	0.334	0.392	0.247	0.320	0.377	0.236
TransH	0.218	0.360	0.043	0.208	0.352	0.038	0.191	0.327	0.032
CKRL(TransH)	0.206	0.339	0.038	0.199	0.334	0.034	0.176	0.309	0.019
NeuRAN(TransH)	0.330	0.380	0.251	0.328	0.378	0.250	0.314	0.371	0.232

Table 9

Ablation study of link prediction results on WN18RR-10% and FB15K237-10%. KGE is TransE

		WN18RR-10%		FB15K237-10%			
	MRR	Hi	t@	MRR	Hi	t@	
		3	1		3	1	
KGE	0.2103	0.3468	0.0333	0.2267	0.2851	0.1067	
KGE + DM	0.2108	0.3476	0.0337	0.2267	0.2848	0.1067	
KGE + RG	0.2134	0.3500	0.0370	0.2268	0.2853	0.1069	
KGE + DIS	0.2203	0.3529	0.0490	0.2723	0.3069	0.1795	
KGE + IRRE	0.3407	0.3925	0.2554	0.2746	0.3030	0.1864	
KGE + ASYM	0.2108	0.3472	0.0341	0.2267	0.2851	0.1067	
KGE + ALL	0.3417	0.3926	0.2562	0.2838	0.3128	0.1987	

Thus we can conclude that implicit axiom information encoded by neural axiom networks helps to improve the quality of learned embeddings of entities and relations and link prediction results. Moreover, such information is more effective on datasets with relatively few relations and triples.

4.5. Ablation study

We conduct ablation studies on link prediction to assess the effectiveness of NeuRAN. As our model is composed of a knowledge graph embedding module and five neural axiom modules, we add each axiom module to the knowledge graph embedding module to investigate the contributions of the axiom module. Specifically, we use the score function and loss function defined in equation (1) and (2) to train our model. TransE is taken as the knowledge graph embedding module. For evaluation, we set the score function as $E(s, r, o) = E_{\text{kge}} + \lambda \cdot E_a$ to illustrate the impact of each axiom module. E(s, r, o) is the score of the triple, and E_{kge} is the score from the knowledge graph embedding module. E_a means the score of the selected axiom and can be $(1 - P_{\text{dm}})$, $(1 - P_{\text{rg}})$, $(1 - P_{\text{dis}})$, $(1 - P_{\text{irr}})$ or $(1 - P_{\text{asy}})$.

From Table 9, we can observe that adding these five axioms can improve link prediction results on WN18RR-10%. The disjoint and irreflexive modules work better than other modules. Notably, the irreflexive axiom module has substantially improved on MRR and Hits@1 metrics. As the number of relations is small and most relations are asymmetric on WN18RR%, using the attention mechanism to aggregate relation representations or adding the asymmetric module has a small gain. For the results on the FB15K237-10% dataset with more relations, the improvement of the disjoint module increases compared to on WN18RR%. Although the domain, range and asymmetric modules are not as efficient as the other modules, we consider them for a comprehensive exploration.

5. Conclusion

In this paper, we propose a novel neural axiom network model which aims to do reasoning on noisy knowledge graphs. We consider encoding not only structural information but also axiom information of triples. Specifically, we propose a knowledge graph embedding module for preserving the structure and five different axiom modules for calculating probability scores that satisfy the corresponding axioms. We evaluate our method on KG noise detection, triple classification and link prediction. Experiments show that axiom information can benefit these tasks.

In the future, we will attempt to explore more implicit or explicit information in triples to enhance the performance of knowledge graph reasoning. Furthermore, we will improve our method to apply it for inconsistency reasoning, as axiom information may be able to provide explanations for inconsistent triples.

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