

Incorporating Global Information in Local Attention for Knowledge Representation Learning

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Abstract

Graph Attention Networks (GATs) have proven a promising model that takes advantage of localized attention mechanism to perform knowledge representation learning (KRL) on graph-structure data, e.g., Knowledge Graphs (KGs). While such approaches model entities' local pairwise importance, they lack the capability to model global importance relative to other entities of KGs. This causes such models to miss critical information in tasks where global information is also a significant component for the task, such as in knowledge representation learning. To address the issue, we allow the proper incorporation of global information into the GAT family of models through the use of scaled entity importance, which is calculated by an attention-based global random walk algorithm. In the context of KRL, incorporating global information boosts performance significantly. Experimental results on KG entity prediction against the state-of-the-arts sufficiently demonstrate the effectiveness of our proposed model.

1 Introduction

Graph Attention Networks (GATs) have been successfully applied to various tasks over graphs (Velickovic et al., 2018; Lee et al., 2018b), such as graph classification (Wu et al., 2019b; Lee et al., 2018a), link prediction (Abu-El-Haija et al., 2018), and node classification (Lee et al., 2019; Zhang et al., 2020a). GATs learn from the underlying graph structure by making use of localized attention mechanism (Wu et al., 2019a; Xu et al., 2019; Vashishth et al., 2020b), where the hidden representation of each node is computed by recursively aggregating and attending over its corresponding local neighbors' features, and the weighting coefficients are calculated inductively with self-attention

strategy (Thekumparampil et al., 2018; Qian et al., 2018; Zhang et al., 2018). The original GATs perform only on single-relational homogeneous graphs (Velickovic et al., 2018; Wang et al., 2019b). Recent advancements were proposed to operate on more general and prevalent multi-relational graphs (Wang et al., 2019b; Hong et al., 2020; Nathani et al., 2019; Zhang et al., 2020c), such as the representative Knowledge Graphs (KGs) which contain multiple types of entities (nodes) and relationships (edges) (Zhou et al., 2018; Han et al., 2018; Wang et al., 2019a; Zhao et al., 2020). However, these approaches can only exploit localized features within the neighborhood of individual entities (Nathani et al., 2019; Busbridge et al., 2019; Zhang et al., 2020c). For some tasks, such simplified localized feature aggregation may be sufficient, but insufficient for knowledge representation learning (KRL) tasks that also need exploring global information (Xie et al., 2020).

In this paper, we concentrate on how to incorporate **global information in local attention** for knowledge representation learning. Specifically, we allow the proper incorporation of global information into the GAT family of models through the use of scaled entity importance, which is estimated by a global random walk algorithm upon the whole graph structural information. In KGs, entity importance¹ indicates the global significance or authority of an entity. Intuitively, it can be quite beneficial if an entity attends more to its "authoritative" neighbors that have high scores of global entity importance. For instance, a movie "Titanic" links to different actors, among which a superstar

¹The notions of its counterparts, e.g., global node importance or object authority, have been widely studied in graphs (Li et al., 2012; Liu et al., 2017; Park et al., 2019), which enable a number of applications such as Web search (Brin and Page, 1998; Kleinberg, 1999), social network analysis (Weng et al., 2010), RecSys (Jing et al., 2014), query disambiguation (Makris et al., 2012; Saxena et al., 2020).

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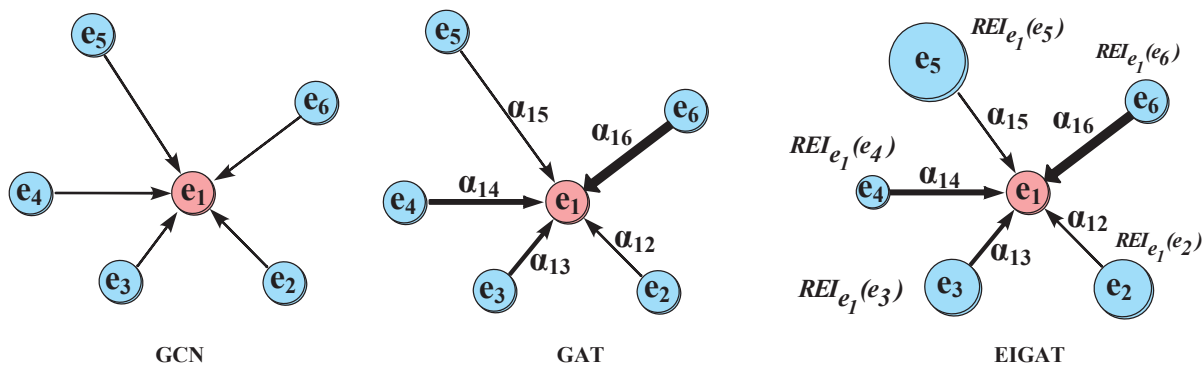


Figure 1: An illustration of Graph Neural Network architectures that model on a graph which is centered on node e_1 with its one-hop neighbors. Left: Graph Convolution Network (GCN); Center: Graph Attention Network (GAT); **Right: our proposed model (EIGAT) that incorporate global information in local attention through the use of relative entity importance (REI).** $REI_{e_1}(e_i)$ is calculated by an attention-based global random walk algorithm upon the whole graph. GAT parameterizes the edge weights based on local attention score (α_{1i} , also represented by the distinct edge widths). Our EIGAT adds the relative importance score (represented by different scaling of nodes), which is derived from global structural information. Note that although relationship should be drawn in the knowledge graph, for clarity, we intentionally ignore it here, which does not hurt the presentation of the basic idea of our model in this paper.

(e.g. “*Leonardo DiCaprio*”) may be more indicative than other actors.

In this paper, we propose a novel Entity Importance-aware Graph Attention Networks, EIGAT, which incorporates global entity importance in local attention mechanism for learning effective knowledge representations. As shown in Figure 1, we give a brief illustration of our proposed EIGAT, which is compared to early proposed GCN (Kipf and Welling, 2017) and GAT (Velickovic et al., 2018). In EIGAT, the importance scores of all entities are expected to be estimated upon global information and to be incorporated in local entity aggregation (Equation 5) for building better entity embeddings. In particular, we provide an attention-based random walk approach to estimate entity importance upon global structural information for serving EIGAT. We conduct extensive experiments on several different types of KGs by entity prediction against state-of-the-art methods, which sufficiently demonstrate our proposed EIGAT can successfully incorporating global information in local attention to improve knowledge representation learning.

The contributions of this paper are threefold:

- We propose to incorporate global information in local attention for knowledge representation learning.
- We propose EIGAT, a novel entity importance-aware graph attention networks which incor-

porate global entity importance into local entity aggregation.

- The extensive experimental results demonstrate the efficacy of our proposed model in link prediction.

2 Related Work

To make this paper self-contained, we introduce some related topics here on Knowledge Representation Learning and Graph Neural Networks (GNNs).

2.1 Knowledge Representation Learning (KRL)

In recent years, knowledge representation learning on KGs has been a hot research topic (Xiao et al., 2017; Shi and Weninger, 2017; Ebisu and Ichise, 2019; Balazevic et al., 2019; Zhang et al., 2020b). These methods roughly fall into four categories: (i) Translational-based models, which view relations as translations from a head entity to a tail entity, such as Trans(E, H, R, D and G) (Bordes et al., 2013; Wang et al., 2014; Lin et al., 2015; Ji et al., 2015; Xiao et al., 2016), ComplEx (Trouillon et al., 2016), JoBi ComplEx (Balkir et al., 2019). (ii) Tensor factorization based models, which assume the score of a triple can be factorized into several tensors, such as RESCAL (Nickel et al., 2011), NTN (Socher et al., 2013), DistMult (Yang et al., 2015), HOLE (Nickel et al., 2016). (iii) CNN-based models, which use convolution over embed-

Table 1: Different variants of Graph Neural Networks: GNN (Scarselli et al., 2008), GCN (Kipf and Welling, 2017), GAT (Velickovic et al., 2018), and our proposed model EIGAT that incorporates global information in local attention.

GNN-based Models	Node Aggregation	Operation	Key Concepts
GNN (Scarselli et al., 2008)	$x_j = f\left(l_j, l_{co[j]}, x_{ne[j]}, l_{ne[j]}\right)$	$f(\cdot)$	Transduction function
GCN (Kipf and Welling, 2017)	$\mathbf{E}^\ell = \sigma\left(\bar{D}^{-\frac{1}{2}} \bar{A} \bar{D}^{-\frac{1}{2}} \mathbf{E}^{\ell-1} W^{\ell-1}\right)$	$\bar{D}^{-\frac{1}{2}} \bar{A} \bar{D}^{-\frac{1}{2}}$	Convolutional operation
GAT (Velickovic et al., 2018)	$\vec{e}_j^\ell = \sigma\left(\sum_{e_i \in In(e_j)} \alpha_{ij}^\ell \cdot W^{\ell-1} \vec{e}_i^{\ell-1}\right)$	α_{ij}	Local attention
EIGAT (our proposed)	$\vec{e}_j^\ell = \sigma\left(\sum_{e_i \in In(e_j)} REI_{e_j}(e_i)^\ell \sum_{k \in \mathcal{R}_{ij}} \alpha_{ikj}^\ell \cdot \vec{v}_{ikj}^\ell\right)$	$REI_{e_j}(e_i), \alpha_{ikj}$	Global information + Local attention

dings to predict links, such as ConvE (Dettmers et al., 2018), ConvKB (Nguyen et al., 2018), InteractE (Vashishth et al., 2020a), ReInceptionE (Xie et al., 2020), and ParamE (Che et al., 2020). (iv) Graph neural network-based models, such as R-GCN (Schlichtkrull et al., 2018), A2N (Bansal et al., 2019), Nathani’s (Nathani et al., 2019), RGhat (Zhang et al., 2020c), ATTH (Chami et al., 2020), which yielded state-of-the-art performance for KRL. Along this line, we focus on a GNN-based approach to deal with knowledge representation learning task.

2.2 Graph Attention Networks (GATs)

Graph Neural Networks (GNNs) develop a deep neural network to deal with arbitrary graphs for representation learning (Scarselli et al., 2008; Zhou et al., 2019; Hou et al., 2020). Graph Convolutional Networks (GCNs) are one of their most prominent progress (Schlichtkrull et al., 2018; Wu et al., 2019a; Xu et al., 2019; Vashishth et al., 2020b), which generalize local convolutional operation on the graph-structured data, i.e. gather information from one-hop neighbors and all neighbors contribute equally in the message passing. Inspired by the successful development of the attention mechanism in NLP and CV, Velickovic et al. (2018) proposed Graph Attention Networks (GATs) by incorporating local attention mechanism (Vaswani et al., 2017; Qian et al., 2018; Lu and Li, 2020) into GCNs, which calculate the hidden states of each node by attending over its neighbors (Thekumparampil et al., 2018; Lee et al., 2018b; Yang et al., 2019).

Recently, several advanced extensions of GATs were proposed for operating on knowledge graphs. Han et al. (2018) proposed to jointly apply attention to KGs and external text data. Busbridge

et al. (2019) proposed RGAT by extending non-relational GATs to incorporate relational information, but with poor performance. Nathani et al. (2019) proposed a triple-level attention model that captures the integrated features of both entity and relation in a given entity’s neighborhood, and Zhang et al. (2020c) proposed a two-level hierarchical attention mechanism. These studies are related to our work in the sense that we all use GNNs to capture more structural information in KGs. However, all of them ignore global information in local attention computation.

Most recently, (Xu et al., 2020) proposed a Transformer-based model to enhance the copy mechanism for abstractive summarization by considering the global importance of each source word based on the degree centrality in the Transformer, which inspires our idea of incorporating global information in local attention for KRL. Table 1 summarizes the key concepts and other different settings of GNNs.

3 Methodology

In this section, we introduce the details of the proposed EIGAT model that incorporates global information in local attention for knowledge representation learning on KGs. We start by describing a single entity importance-aware graph attention layer, which is the building block of our model’s overall architecture. Before that, we briefly introduce the notations of this paper.

Notations. In a graph attention networks with L layers, the input to ℓ -th layer ($\ell = 1, \dots, L$) are two embedding sets: (1) the *output entity embeddings* from $(\ell-1)$ -th layer which is represented by a matrix $\mathbf{E}^{\ell-1} \in \mathbb{R}^{\eta^{\ell-1} \times N_e}$, $\mathbf{E}^{\ell-1} = \{\vec{e}_1^{\ell-1}, \vec{e}_2^{\ell-1}, \dots, \vec{e}_{N_e}^{\ell-1}\}$, where N_e is the num-

ber of entities, and $\eta^{\ell-1}$ is the dimension of output entity embedding in $(\ell-1)$ -th layer. **(2)** the *output relationship embeddings* from $(\ell-1)$ -th layer, denoted by a matrix $\mathbf{R}^{\ell-1} \in \mathbb{R}^{\zeta^{\ell-1} \times N_r}$, $\mathbf{R}^{\ell-1} = \{\vec{\mathbf{r}}_1^{\ell-1}, \vec{\mathbf{r}}_2^{\ell-1}, \dots, \vec{\mathbf{r}}_{N_r}^{\ell-1}\}$, where N_r and $\zeta^{\ell-1}$ represent the number of relationships and the output relationship’s feature dimension in $(\ell-1)$ -th layer, respectively. The ℓ -th layer then produces the corresponding new output embedding matrices (of potentially different cardinality), $\mathbf{E}^\ell \in \mathbb{R}^{\eta^\ell \times N_e}$ and $\mathbf{R}^\ell \in \mathbb{R}^{\zeta^\ell \times N_r}$. Specifically, we describe the ℓ -th graph attention layer.

3.1 Local Attention Evaluation

A triple relation $t_{ij}^k = (e_i \xrightarrow{r_k} e_j)$ indicates a relationship r_k between head entity e_i and tail entity e_j . Following (Nathani et al., 2019), the representation $\vec{\mathbf{v}}_{ikj}^\ell$ of the triple t_{ij}^k is built as follows:

$$\vec{\mathbf{v}}_{ikj}^\ell = \mathbf{W}_1^\ell \cdot [\vec{\mathbf{e}}_i^{\ell-1} \parallel \vec{\mathbf{r}}_k^{\ell-1} \parallel \vec{\mathbf{e}}_j^{\ell-1}], \quad (1)$$

where \mathbf{W}_1^ℓ denotes a linear transformation matrix in ℓ -th layer, $\vec{\mathbf{e}}_i^{\ell-1}$, $\vec{\mathbf{r}}_k^{\ell-1}$ and $\vec{\mathbf{e}}_j^{\ell-1}$ denote the output embeddings of e_i , r_k and e_j in $(\ell-1)$ -th layer, respectively. \parallel represents concatenation. We then calculate the absolute relation attention value b_{ikj}^ℓ of the triple t_{ij}^k .

$$b_{ikj}^\ell = \text{LeakyReLU}\left(\mathbf{W}_2^\ell \cdot \vec{\mathbf{v}}_{ikj}^\ell\right), \quad (2)$$

where \mathbf{W}_2^ℓ and LeakyReLU are a linear weight vector in ℓ -th layer and a non-linearity active function respectively that act upon the embedding $\vec{\mathbf{v}}_{ikj}^\ell$ in turn. We then utilize *softmax* to evaluate the relative relation attention value α_{ikj}^ℓ of the triple t_{ij}^k in ℓ -th layer.

$$\alpha_{ikj}^\ell = \text{softmax}_{ik}(b_{ikj}^\ell) = \frac{\exp\{b_{ikj}^\ell\}}{\sum_{e_n \in \text{In}(e_j)} \sum_{r \in \mathcal{R}_{nj}} \exp\{b_{nrj}^\ell\}}. \quad (3)$$

$\text{In}(e_j)$ denotes the neighbors pointing to targeted tail entity e_j , \mathcal{R}_{nj} denotes the set of relationships between e_n and e_j .

3.2 Global Entity Importance Estimation

To obtain global entity importance $EI(e_i)$ of an entity e_i , we formally introduce a relation attention-based global random walk method, as follows:

$$EI(e_i)^t = (1-d) + d \times \sum_{e_m \in \text{In}(e_i)} \sum_{r \in \mathcal{R}_{mi}} \frac{b_{mri}}{\sum_{e_n \in \text{Out}(e_m)} \sum_{\bar{r} \in \mathcal{R}_{mn}} b_{m\bar{r}n}} EI(e_m)^{t-1}, \quad (4)$$

where d is a hyperparameter denoting the probability that an imaginary surfer randomly moves to a neighboring entity. $(1-d)$ denotes the probability of teleporting to any other entities randomly, which is able to alleviate the *information island problem* caused by the isolated entities that lack of any in-degree or out-degree neighbors (e.g. #median in-degree=0 in NELL-995 in Table 2). $\text{Out}(e_m)$ denotes the neighborhoods that an entity e_m points to. $EI(e_m)^{t-1}$ denotes the EI score of the entity e_m in $(t-1)$ -th iteration. The random walk distance² t depends on both the number of attention layers L and training epochs C , $t \in (1, L \times C]$. The relation weights (e.g. b_{mri}) are calculated by Equation (2). Unlike conventional fixed weights-based random walk methods (Mihalcea and Tarau, 2004; Florescu and Caragea, 2017), a novelty is that the dynamic relation weights (e.g. b_{mri}) are iteratively and automatically optimized during training by the graph attention mechanism. In line with the theoretical desiderata for modeling node importance in MRGs, this method develops the following essential characteristics: **(i) Neighborhood-awareness**, i.e. neighboring EI scores can be taken into account when a given entity’s importance score is modeled. **(ii) Relationship-awareness**, i.e. different relationships could play a different role in propagating EI score. **(iii) Centrality-awareness**, i.e. more central nodes inherently and reasonably would be more important than less central nodes. **(iv) Universal and flexible**, i.e. it utilizes only graph global structural information.

3.3 Incorporate Global Information in Local Attention

Though attention mechanism can assign different importance to nodes via learned weights, it is still a local computation. The attention value, e.g., α_{ikj} in Equation (3), is the function of pairwise feature interaction within local neighborhood and do not take account of entity importance from global graph structure. To this end, we incorporate global information in local attention computation, as shown in Figure 1 (EIGAT).

Specifically, to generate the output embedding $\vec{\mathbf{e}}_j^\ell$ of tail entity e_j in ℓ -th layer, we incorporate global relative head entity importance $REI_{e_j}(e_i)^\ell$ in local attention to conduct entity aggregation with its associated triple representations $\vec{\mathbf{v}}_{ikj}^\ell$ weighted

²To denote EI score of e_i in ℓ -th layer explicitly, we omit the training epoch symbol and denote it as $EI(e_i)^\ell$ in the following.

by their relative attention values α_{ikj}^ℓ , as follows:

$$\vec{e}_j^\ell = \sigma \left(\sum_{e_i \in In(e_j)} REI_{e_j}(e_i)^\ell \sum_{k \in \mathcal{R}_{ij}} \alpha_{ikj}^\ell \cdot \vec{v}_{ikj}^\ell \right), \quad (5)$$

and

$$\begin{aligned} REI_{e_j}(e_i)^\ell &= \text{softmax}_{In(e_j)}(EI(e_i)^\ell) \\ &= \frac{\exp\{EI(e_i)^\ell\}}{\sum_{e'_i \in In(e_j)} \exp\{EI(e'_i)^\ell\}}, \forall e_i \in In(e_j). \end{aligned} \quad (6)$$

In Eq. (5), we bring in global relative entity importance $REI_{e_j}(e_i)^\ell$ of different head entities in $In(e_j)$ for learning more about those significant neighboring entities, and thus could get better knowledge representations for the targeted tail entity e_j .

To stabilize the learning process of self-attention, as suggested by (Velickovic et al., 2018), we employ multi-head attention. Specifically, M independent attention mechanisms execute the transformation of Eq. (5), and then their features are concatenated as:

$$\vec{e}_j^\ell = \left\| \sum_{m=1}^M \sigma \left(\sum_{e_i \in In(e_j)} REI_{e_j}(e_i)^{\ell,m} \sum_{k \in \mathcal{R}_{ij}} \alpha_{ikj}^{\ell,m} \cdot \vec{v}_{ikj}^{\ell,m} \right) \right\| \quad (7)$$

We conduct a linear transformation on input relationship embedding $\vec{r}_k^{\ell-1} \in \mathbb{R}^{\zeta^{\ell-1}}$ in ℓ -th layer as:

$$\vec{r}_k^\ell = \mathbf{W}^{\ell, \mathcal{R}} \cdot \vec{r}_k^{\ell-1}, \quad (8)$$

where $\mathbf{W}^{\ell, \mathcal{R}} \in \mathbb{R}^{\zeta^\ell \times \zeta^{\ell-1}}$ is a weight matrix, $\zeta^{\ell-1}$ and ζ^ℓ are dimensions of input and output relationship embeddings, respectively. $\vec{r}_k^\ell \in \mathbb{R}^{\zeta^\ell}$ represents the output relationship embedding in the ℓ -th layer.

4 Model Architecture

Our model follows an encoder-decoder framework: **(i)** the encoder model includes L attention layers, **(ii)** the decoder model provides a scoring function (Eq. 11) to calculate the likelihood of given triples being valid. Based on it, the KG incompleteness issue is expected to be alleviated by link prediction (Section 5), i.e., inferring possible missing relations, e.g. $(e_i, r_k, ?)$ or $(?, r_k, e_j)$.

4.1 Encoder

Based on a single attention layer introduced above, we build the overall architecture of our encoder model with L layers. In practice, we set $L=2$ for

our encoder model. In the final L -th layer, instead of concatenation (Equation 7), we employ averaging and delay applying the final non-linearity activation:

$$\begin{aligned} \vec{e}_j^L &= \\ \sigma \left(\frac{1}{M} \sum_{m=1}^M \sum_{e_i \in In(e_j)} REI_{e_j}(e_i)^{L,m} \sum_{k \in \mathcal{R}_{ij}} \alpha_{ikj}^m \vec{v}_{ikj}^{L,m} \right) \end{aligned} \quad (9)$$

To keep initial entity information in the final embedding, we obtain the final entity embedding $\vec{e}^* \in \mathbb{R}^{\eta^L}$ by combining the transformed initial embeddings $\vec{e}^0 \in \mathbb{R}^{\eta^0}$ and the output entity embedding $\vec{e}^L \in \mathbb{R}^{\eta^L}$ of the L -th layer, as follows:

$$\vec{e}^* = \mathbf{W}^* \cdot \vec{e}^0 + \vec{e}^L, \quad \forall e \in \mathcal{E}. \quad (10)$$

$\mathbf{W}^* \in \mathbb{R}^{\eta^L \times \eta^0}$ is a projecting matrix. The initial entity embeddings (i.e. $\vec{e}^0, \forall e \in \mathcal{E}$) and relationship embeddings (i.e. $\vec{r}^0, \forall r \in \mathcal{R}$) are pre-trained by Bordes et al. (2013).

4.2 Decoder

Among the existing KG completion (KGC) models, we utilize the most recent model ConvKB (Nguyen et al., 2018) as decoder model³. Given a triple t_{ij}^k , the scoring function is formally defined as:

$$f(t_{ij}^k) = \left(\left\| \sum_{m=1}^{|\Omega|} g([\vec{e}_i^*, \vec{r}_k^L, \vec{e}_j^*] * \omega^m) \right\| \right) \cdot \mathbf{W}, \quad (11)$$

where Ω denotes the set of filters, $\tau=|\Omega|$ and $\omega \in \Omega$. Ω and \mathbf{W} are shared parameters and independent of e_i, r_k and e_j . $g(\cdot)$ is an activation function such as ReLU. $*$ denotes a convolution operator. These τ feature maps are concatenated into a single vector $\in \mathbb{R}^{\tau\phi}$ which is then computed with a weight vector $\mathbf{W} \in \mathbb{R}^{\tau\phi}$ via a dot product to give a likelihood score for the triple t_{ij}^k . ϕ denotes the dimension of entity and relation embeddings. In practice, we set $\phi=\eta^L=\zeta^L$ for ConvKB.

4.3 Optimization

We utilize a two-step training procedure for the encoder-decoder framework, which is a routine optimization way for it (Zhou et al., 2019). **(i)** We first train the encoder model to learn the embeddings of entities and relationships, by minimizing

³We choose ConvKB here, and it is not difficult for other KGC methods, such as CapsE (Nguyen et al., 2019), ConvE (Dettmers et al., 2018), etc. Note that we also tried different models as decoder, but found that ConvKB performs best.

Table 2: Statistics of datasets.

Datasets	#Entities	#Rel	#Edges				Mean in-degree	Median in-degree	Density
			Train	Validation	Test	Total			
Kinship	104	25	8544	1068	1074	10,686	82.15	82.5	0.998
FB15k-237	14,541	237	272,115	17,535	20,466	310,116	18.71	8	0.001
NELL-995	75,492	200	149,678	543	3992	154,213	1.98	0	2.71E-5

a hinge-loss function, as follows:

$$\mathcal{L}_1 = \sum_{t_{ij}^k \in \mathcal{G}} \sum_{t_{ij}^{k'} \in \mathcal{G}'} \max \{ h_{t_{ij}^{k'}} - h_{t_{ij}^k} + \gamma, 0 \}. \quad (12)$$

Here, $h_{t_{ij}^k} = \|\mathbf{e}_i^* + \mathbf{r}_k^L - \mathbf{e}_j^*\|_{\ell_1}$ indicates the translational scoring function of the triple t_{ij}^k (Bordes et al., 2013). $\gamma > 0$ is a margin hyper-parameter.

(ii) We then train and learn the parameters of the decoder model ConvKB for link prediction, by minimizing a soft-margin loss function, as follows:

$$\mathcal{L}_2 = \sum_{t_{ij}^k \in \{\mathcal{G} \cup \mathcal{G}'\}} \log \left(1 + \exp \left(l_{t_{ij}^k} \cdot f(t_{ij}^k) \right) \right) + \lambda \|\mathbf{W}\|_2^2, \quad (13)$$

in which, $l_{t_{ij}^k} = \begin{cases} 1, & t_{ij}^k \in \mathcal{G} \\ -1, & t_{ij}^k \in \mathcal{G}' \end{cases}$. \mathcal{G} and \mathcal{G}' are the sets of positive triples and negative triples, respectively.

$$\mathcal{G}' = \{t_{i'j}^k | e_i' \in \mathcal{E} \setminus e_i\} \cup \{t_{ij}^{k'} | e_j' \in \mathcal{E} \setminus e_j\}. \quad (14)$$

5 Experiments

We evaluate the effectiveness of our proposed model EIGAT by link prediction (determined by Equation 11), which aims to infer possible missing relations, i.e., predict e_j given $(e_i, r_k, ?)$ or predict e_i given $(?, r_k, e_j)$.

5.1 Datasets

We use three public benchmark datasets for link prediction experiments, including: *Kinship* (Lin et al., 2018), *NELL-995* (Xiong et al., 2017), *FB15K-237* (Toutanova et al., 2015), where we discard another popular dataset *WN18RR* due to its too sparse to learn global information. The basic statistics of all datasets are included in Table 2. To explore the performance of our proposed model on different datasets with different global topology characteristics, we compute their density value (Coleman and Moré, 1983) and report them in Table 2. Since the densities in *NELL-995* is sparser than *Kinship* and *FB15K-237*, and its median in-degree even is 0, it is relative hard for global entity importance estimation in *NELL-995*.

Definition 1. (Graph Density). Graph density aims to measure how sparse a graph is. Similar to (Coleman and Moré, 1983), given a graph \mathcal{G} , it's formally defined as follows:

$$D(\mathcal{G}) = \frac{E}{N(N-1)}, \quad (15)$$

where N denotes the number of nodes in \mathcal{G} , and E denotes the number of edges in \mathcal{G} . The lower the $D(\mathcal{G})$, the sparser the graph is.

Table 3: Hyperparameters for the encoder model EIGAT on all datasets.

Datasets	Kinship	NELL-995	FB15k-237
Learning rate	1e-2	1e-3	1e-3
Weight decay	1e-6	1e-6	1e-6
Epochs	4000	3000	3200
Dropouts	0.3	0.5	0.5
Leaky Relu	0.2	0.2	0.2
nheads	2	2	2
Final dimensions	200	200	200
Negative ratio	2	2	2
Margin	1	1	1
RW parameter d	0.85	0.85	0.85

Table 4: Hyperparameters for the decoder model EIGAT on all datasets.

Datasets	Kinship	NELL-995	FB15k-237
Learning rate	1e-2	1e-3	1e-3
Weight decay	1e-5	5e-6	5e-7
Epochs	400	200	200
Dropouts	0.0	0.3	0.2
Filters	50	400	50

5.2 Baselines

To demonstrate the effectiveness of our proposed model EIGAT for link prediction, we compare it with the following state-of-the-art (SOTA) baselines:

- TransE (Bordes et al., 2013): a most widely used and early KGC models.
- DistMult (Yang et al., 2015): a popular tensor factorization-based KGC model which uses a bi-linear scoring function to calculate knowledge triples' scores.

Table 5: **Link prediction results** on *Kinship* and *NELL-995*. The results of baselines are directly taken from the original papers. The best scores are in **bold**.

	Kinship					NELL-995				
	MR	MRR	Hits@N (%)			MR	MRR	Hits@N (%)		
			@1	@3	@10			@1	@3	@10
TransE (Bordes et al., 2013)	6.8	0.309	0.9	64.3	84.1	2100	0.401	34.4	47.2	50.1
DistMult (Yang et al., 2015)	5.26	0.516	36.7	58.1	86.7	4213	0.485	40.1	52.4	61
ComplEx (Trouillon et al., 2016)	2.48	0.823	73.3	89.9	97.11	4600	0.482	39.9	52.8	60.6
ConvE (Dettmers et al., 2018)	2.03	0.833	73.8	91.7	98.14	3560	0.491	40.3	53.1	61.3
ConvKB (Nguyen et al., 2018)	3.3	0.614	43.62	75.5	95.3	600	0.43	37.0	47	54.5
R-GCN (Schlichtkrull et al., 2018)	25.92	0.109	3	8.8	23.9	7600	0.12	8.2	12.6	18.8
Nathani’s (Nathani et al., 2019)	1.94	0.904	85.9	94.1	98	965	0.530	44.7	56.4	69.5
EIGAT (Ours)	1.66	0.963	94.8	96.6	98.4	1210	0.545	46.4	58.4	71.5

- ComplEx (Trouillon et al., 2016): an advanced extension of DistMult which encodes entities and relationships into complex vector space instead of real-valued vector space.
- ConvE (Dettmers et al., 2018): a popular convolutional network-based KGC model.
- ConvKB (Nguyen et al., 2018): another SOTA convolutional network-based KGC model.
- R-GCN (Schlichtkrull et al., 2018): an advanced extension of GCN that can effectively model multi-relational data.
- Nathani’s (Nathani et al., 2019): a recent KGC model that models the local neighborhood via graph relational attention network.
- A2N (Bansal et al., 2019): a recent model that learns query-dependent representations of entities based on a GNN structure.
- HAKE (Zhang et al., 2020b): a SOTA KGC model that models semantic hierarchies
- InteractE (Vashishth et al., 2020a): a recent extension of ConvE that increase the interaction between relation and entity embeddings.
- ReInceptionE (Xie et al., 2020): a recent extension of ConvE that uses local-global structural information.
- ParamE (Che et al., 2020): another extension of ConvE that use relation embeddings.
- ATTH (Chami et al., 2020): a SOTA model that use hyperbolic space and attention-based geometric transformation.

- RGHAT (Zhang et al., 2020c): a SOTA KGC model that models the local neighborhood via hierarchical attention mechanism.

5.3 Evaluation Protocol

We utilize ranking criteria for evaluation. For each testing triple, we remove the head entity or tail entity and replace it by each of the entities in \mathcal{E} in turn. The model scores of the corrupted triples would be computed by the decoder model (Eq. 11) and then sorted by descending order. We can obtain the exact rank of the correct triple in the candidates. Similar to most baselines, we report the experimental results in “Filter” setting, i.e. removing corrupted triples that are already present in datasets during ranking. The evaluation metrics include: the mean reciprocal rank (MRR), mean rank (MR), and the proportion of correct entities ranked in the top N (HITS@N, N=1, 3, 10).

5.4 Training Protocol

Table 3 and Table 4 report the detailed hyperparameter settings of encoder and decoder models for EIGAT, respectively. In the training, we set M=2 heads attention mechanism. The final dimensions of entity and relation embeddings are set to 200. The slop parameter α of LeakyReLU in Eq. (2) is set as 0.2 on all datasets. We use auxiliary relations from 2-hop neighborhood to aggregate more information about the neighborhoods. EI scores are initialized randomly in (0,1). We utilize a typical value for $d = 0.85$ (Mihalcea and Tarau, 2004; Florescu and Caragea, 2017).

5.5 Results and Analysis

Table 5 and Table 6 demonstrate the results of link prediction (significance level of 0.05). We can observe that: (i) The results clearly indicate that

Table 6: **Link prediction results** on *FB15K-237*. The results of baselines are directly taken from the original papers. The best scores are in **bold**.

	FB15K-237				
	MR	MRR	Hits@N (%)		
			@1	@3	@10
TransE (Bordes et al., 2013)	323	0.279	19.8	37.6	44.1
DistMult (Yang et al., 2015)	512	0.281	19.9	30.1	44.6
ComplEx (Trouillon et al., 2016)	546	0.278	19.4	29.7	45
ConvE (Dettmers et al., 2018)	245	0.312	22.5	34.1	49.7
ConvKB (Nguyen et al., 2018)	216	0.289	19.8	32.4	47.1
R-GCN (Schlichtkrull et al., 2018)	600	0.164	10	18.1	30
ATTH (Chami et al., 2020)	-	0.348	25.2	38.4	54.0
HAKE (Zhang et al., 2020b)	-	0.346	25.0	38.1	54.2
InteractE (Vashishth et al., 2020a)	172	0.354	26.3	-	53.5
ReInceptionE (Xie et al., 2020)	173	0.349	-	-	52.8
ParamE (Che et al., 2020)	-	0.399	31.0	43.8	57.6
RGHAT (Zhang et al., 2020c)	196	0.522	46.2	54.6	63.1
EIGAT (Ours)	154	0.541	47.6	57.1	66.1

EIGAT significantly and consistently outperforms all state-of-the-art baselines on most metrics in all benchmark datasets, which demonstrate the effectiveness of our proposed model. (ii) The advantages EIGAT compared to baselines on *NELL-995* seem to be smaller than others. It is because that rich global structural information in relative dense graphs, i.e., *Kinship*, and *FB15K-237*, leads to more effective entity importance estimation by global random walk methods, comparing with less global structural knowledge in relative sparse graphs, i.e., *NELL-995*. The results demonstrate *NELL-995* is more difficult than others for EIGAT to learn, but the comparable results also verify the effectiveness and robustness of our model on both scenarios.

5.6 Ablation Study

To analyze the behavior of global information in EIGAT, we compare EIGAT with EIGAT-Remove-global (i.e., removing global entity importance from EIGAT). The comparison results in Table 7 indicate that EIGAT achieves improvements against EIGAT-Remove-global on all metrics. In particular, on MR, EIGAT surpasses EIGAT-Remove-global by a large margin 56. The results demonstrate our model can successfully take account of global information in local attention to aggregate more effective entity representations.

5.7 Case Study

Table 8 gives examples of entity prediction results of EIGAT on the FB15k-237 testing set (predicting tail entities). This illustrates the efficacy of our proposed EIGAT. Given a head entity and a relation, the top predicted tail entities (and the true one) are

Table 7: **Ablation Study**. Link prediction results by different variants of our model on *FB15K-237*.

	FB15K-237				
	MR	MRR	Hits@N (%)		
			@1	@3	@10
EIGAT-Remove-global	210	0.518	46	54	62.6
EIGAT	154	0.541	47.6	57.1	66.1

depicted. Even if the true fact is not always at the best front, the predicted results can still reflect common-sense.

Table 8: Example predictions on the FB15K-237 test set using EIGAT. **Bold** indicates the test triplet’s true tail and italics other true tails present in the training set.

Head Entity	Relation	Tail Entities
X-Men	production companies	Marvel Entertainment , DC Comics, 20th Century Studios, American Zoetrope
United States of America	form of government	<i>presidential régime</i> , Democracy, republic , parliamentary monarchy, parliamentary system
Belgium	time zones	Central European Time , Atlantic Time Zone, Belgium

6 Conclusion and Future Work

In this paper, we propose to incorporate global information in local attention for knowledge representation learning and introduce a novel GAT-based model that incorporates global entity importance. In particular, we provide an attention-based global random walk approach to estimate entity importance. The experimental results of entity prediction demonstrate that our model can successfully take into account global information in local attention to improve knowledge representation learning. Interesting future work directions include generalizing EIGAT to other relational graphs (e.g. heterogeneous information network (HIN), user-item graph in recommendation system), and exploring an advanced variant of EIGAT in a semi-supervised learning scenario.

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