Swift and Sure: Hardness-aware Contrastive Learning for Low-dimensional Knowledge Graph Embeddings

Kai Wang∗
School of Software, the Key Laboratory for Ubiquitous Network and Service Software of Liaoning Province, Dalian University of Technology
Dalian, Liaoning, China
kai_wang@mail.dlut.edu.cn

Yu Liu
School of Software, the Key Laboratory for Ubiquitous Network and Service Software of Liaoning Province, Dalian University of Technology
Dalian, Liaoning, China
yuliu@dlut.edu.cn

Quan Z. Sheng
Intelligent Computing Laboratory
School of Computing
Macquarie University
Sydney, NSW, Australia
michael.sheng@mq.edu.au

ABSTRACT
Knowledge graph embedding (KGE) has drawn great attention due to its potential in automatic knowledge graph (KG) completion and knowledge-driven tasks. However, recent KGE models suffer from high training cost and large storage space, thus limiting their practicality in real-world applications. To address this challenge, based on the latest findings in the field of Contrastive Learning, we propose a novel KGE training framework called Hardness-aware Low-dimensional Embedding (HaLE). Instead of the traditional Negative Sampling, we design a new loss function based on query sampling that can balance two important training targets, Alignment and Uniformity. Furthermore, we analyze the hardness-aware ability of recent low-dimensional hyperbolic models and propose a lightweight hardness-aware activation mechanism, which can help the KGE models focus on hard instances and speed up convergence. The experimental results show that in the limited training time, HaLE can effectively improve the performance and training speed of KGE models on five commonly-used datasets. The HaLE-trained models can obtain a high prediction accuracy after training few minutes and are competitive compared to the state-of-the-art models in both low- and high-dimensional conditions.

CCS CONCEPTS
• Computing methodologies → Knowledge representation and reasoning; • Information systems → Entity relationship models.

KEYWORDS
Knowledge Graph Embedding, Contrastive Learning, Link Prediction, Knowledge Graph

∗Corresponding author

Permission to make digital or hard copies of all or part of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. Copyrights for components of this work owned by others than ACM must be honored. Abstracting with credit is permitted. To copy otherwise, or republish, to post on servers or to redistribute to lists, requires prior specific permission and/or a fee. Request permissions from permissions@acm.org.

WWW'22, April 25–29, 2022, Lyon, France
© 2022 Association for Computing Machinery.
ACM ISBN 978-1-4503-XXXX-X/18/06. . $15.00
https://doi.org/10.1145/1122445.1122456

ACM Reference Format:
Kai Wang, Yu Liu, and Quan Z. Sheng. 2022. Swift and Sure: Hardness-aware Contrastive Learning for Low-dimensional Knowledge Graph Embeddings. In WWW '22: Proceedings of The ACM Web Conference, April 25–29, 2022, Lyon, France. ACM, New York, NY, USA, 10 pages. https://doi.org/10.1145/1122445.1122456

1 INTRODUCTION
Knowledge Graph Embedding (KGE) represents entities and relations of knowledge graphs (KGs) in the semantic vector space, and has shown great potential in automatic KG completion and knowledge-driven tasks [15, 16, 31, 33]. Given a query having an entity and the relation of a triple, a typical KGE model learns embedding vectors by predicting the missing entity from the whole entity set [30]. However, the existing KGE models have limited practicality in real-world applications [19, 23]. To improve the prediction accuracy, recent KGE models utilize complicated computational structures and high-dimensional vectors up to 500 or even 1,000 dimensions [7, 12, 22]. Training such high-dimensional models demands prohibitive training costs and storage space, yet only achieving slight performance increase. Meanwhile, large-scale KGs in real-world industrial applications, usually contain millions or billions of entities and need to be updated constantly based on real-time business data. Consequently, current KGE models mostly still stay in laboratory environments and remain difficult to be deployed in practical applications [17, 29].

To reduce the training costs, a promising way is to design new loss functions. As the Negative Sampling loss has been indicated time-consuming and unstable, Sun et al. [22] proposed a Self-adversarial Negative Sampling loss, which uses the Softmax-normalized triple score as the weight of each negative sample to accelerate model convergence. Besides, recent research efforts from the community have proposed several non-sampling training strategies in All-Negative or Non-Negative ways [10, 14]. Unfortunately, these methods still have respective constraints and can only be applied to some specific KGE models. To reduce the space complexity, low-dimensional hyperbolic-based KGE models have drawn attention, such as MuRP, RoTH, ReH and AtH [2, 5]. Although they can achieve good performance when using 32 or 64 dimensions, the calculations in the hyperbolic space are much more complicated than those in the Euclidean space [28].

Several valuable insights from the latest Contrastive Learning studies, inspire us to analyze these previous KGE work from...
a new perspective. Wang and Isola [32] proved that two key properties, Alignment and Uniformity, determine the performance of Contrastive Learning methods. Except aligning the features of positive pairs, the CL method trains negative samples to uniformize the local feature distribution, such that separable features can be learned. Besides, Wang and Liu [27] further proposed that the contrastive loss is a hardness-aware loss function, because the temperature $r$ can control the strength of penalties on different negative samples. These insights motivate us to re-think the training target of KGE models. First, to better separate positive and negative triples, Negative Sampling and non-sampling strategies in KGE models can be seen as to achieve uniformity. Second, to adjust the contributions of different samples, similar attempts have been made in the self-adversarial loss [22] and recent hyperbolic KGE models. We find that the nonlinear function in the hyperbolic geometry can give the hardness-aware ability to the hyperbolic models.

In this paper, we propose a novel KGE training framework, Hardness-aware Low-dimensional Embedding (HaLE). To the best of our knowledge, our work is the first to connect the Contrastive Learning and KGE models. In the HaLE framework, we propose two major innovative techniques: the Query Sampling Loss and the Hardness-aware Activation Mechanism. To balance the two properties, Alignment and Uniformity, the new loss function maximizes the scores of all positive instances, while forcing all entity vectors to stay away from a limited number of sampled query vectors in the vector space. As the result, the Query Sampling loss can provide stable gradients with small training costs. Furthermore, we propose the Hardness-aware Activation mechanism with novel activation functions, Hanon($\cdot$) and Halin($\cdot$), to flexibly control the strength of penalties of easy and difficult instances. Requiring fewer calculations, this mechanism can replace the role of hyperbolic geometry in the recent state-of-the-art hyperbolic models. We conduct extensive experiments on five commonly-used datasets, including FB15k-237, WN18RR, CoDex-S/M/L. The results show that HaLE can significantly improve the training speed of multiple KGE models. Compared with previous KGE training strategies, the HaLE-trained models can obtain a higher prediction accuracy after training several minutes. Their performance is competitive compared to the state-of-the-art KGE models in both low- and high-dimensional conditions.

The rest of the paper is organized as follows. We introduce the background and notations in Section 2. Section 3 details the HaLE framework and its two main components. Section 4 reports the experimental studies, and Section 5 further discusses the related work. Finally, we provide some concluding remarks in Section 6.

2 BACKGROUND
In this section, we will briefly describe the Knowledge Graph Embedding and the Contrastive Learning techniques. Table 1 introduces the main notations that will be used in this paper.

### 2.1 Knowledge Graph Embedding
A Knowledge Graph $G$ is composed by a collection of triples $(e_h, r, e_t)$, in which $r \in R$ is the relation between the head and tail entities $e_h, e_t \in E$. A KGE model is usually trained by the link prediction task to represent each entity $e \in E$ (or relation $r \in R$) as a d-dimensional continuous vector. Given a query $q = (e, r)$, link prediction aims to find the target entities $e_p \in E$ satisfying that $(e, r, e_p)$ or $(e_p, r, e)$ belongs to the knowledge graph $G$.

To achieve this goal, the KGE model needs to score all candidate triples via a scoring function. Given a triple $(e_h, r, e_t)$, the mainstream scoring function can be defined as $f(e_h, r, e_t) = \Psi(e_h, e_t)$, which involves the following two operations:

- **Transform function** $\Phi(e_h, r)$ transforms the head vector $e_h$ using the relation vector $r$ and outputs the query vector $q$.
- **Similarity function** $\Psi(q, e_t)$ measures the similarity between the tail vector $e_t$ and the transformed head vector $q$.

Taken two typical KGE models, TransE [3] and DistMult [34], as examples, TransE’s transform function is $\Phi(e_h, r) = e_h + r$ and its similarity function is equivalent to the $L_1$ or $L_2$ distance, while the transform function of DistMult is $\Phi(e_h, r) = e_h \cdot r$ and its similarity function is the dot product operation. The similarity score $s$ produced by the scoring function $f(\cdot)$ is regarded as the triple score. Most KGE models are trained by minimizing a Negative Sampling loss, to make the score of the qualified triple higher than those of negative samples.

### 2.2 Contrastive Learning
Contrastive Learning (CL) has achieved remarkable success in unsupervised representation learning for image and sequential data [6]. Without human supervision, Contrastive Learning methods attempt to learn the invariant representation of different views of the same instance by attracting positive pairs and separating negative pairs. Given a training set of positive pairs $D_{pos}$, a common design of the contrastive loss is formulated as:

$$L_{\text{cont}} = \mathbb{E} \left[ -\log \frac{\exp(f(x_j, x_j')/\tau)}{\sum_k \exp(f(x_j, x_k')/\tau) + \exp(f(x_j, x_j')/\tau)} \right],$$

where $(x_j, x_j') \in D_{pos}$, $f(\cdot)$ is the similarity function, and $(x')$ is the sampled negative instances. This loss form is similar to the cross-entropy loss function. The temperature $\tau$ is a hyper-parameter to help discriminate positive and negative samples.
Essentially, both KGE and CL aim to learn representations without human supervision. They define the positive and negative instances for each sample, and learn representation vectors to better discriminate them. To learn the invariant representation of an image or a sentence, a CL method first generates different views of each sample as positive instances via data augmentation technologies. Then it trains the encoder to make the features of these positive instances more similar, and meanwhile separates them from the features of the other negative instances. Training a KGE model follows a similar process. Given an existing triple \((e_p, r, e_t)\), the query \(q = (e_p, r)\) can be regarded as a positive instance of \(e_t\). The KGE model assigns the positive triple an optimal score, which is equivalent to making the query vector \(q\) more similar to \(e_t\) than those of the other entities. Hence, from the perspective of Contrastive Learning, we obtain a new understanding of the KGE problem. Given an entity \(e\) and its related triples in \(G\), the \(e\)-r queries from these triples can be regarded as multiple positive versions of the center entity \(e\). Similar as CL methods, a KGE model has two targets, aligning the entity vector with its query vectors and separating them with the other entity vectors.

3 METHODOLOGY

Because of the commonality between KGE and Contrastive Learning (CL), we exploit the newest findings of the CL mechanism to understand and improve the KGE training procedure. Based on the specific characteristics of KGs, we propose a novel training strategy for KGE models, namely Hardness-aware Low-dimensional Embedding (HaLE). Although the Negative Sampling loss is widely used in previous KGE and CL methods, the sampled negative instances bring uncertainty into KGE training. Therefore, we propose a new Query Sampling loss to achieve both Alignment and Uniformity, which will be detailed in Sec. 3.1. To achieve the hardness-aware ability like the temperature mechanism in CL, we propose a novel Hardness-aware Activation mechanism in Sec. 3.2. Our mechanism can adjust the contributions of instances according to their degrees of hardness. Finally, the whole HaLE framework and several HaLE-based KGE models are described in Sec. 3.3.

3.1 Query Sampling Loss

Negative sampling has been proved effective and widely used to learn KG embedding and word embedding [3, 11]. Only considering a subset of negative instances, Negative Sampling helps reduce the time complexity of one training epoch. However, randomly sampling negative instances for each triple requires additional training time, especially for large-scale KGs. The uncertainty in the sampling procedure brings fluctuations into KGE training and impedes model convergence. To omit Negative Sampling, recent work proposed two representative non-sampling approaches, i.e., All-Negative training and Non-Negative training [10, 14]. The general loss functions of the two approaches are as follows:

\[
\mathcal{L}_{\text{allneg}}(T) = \mathbb{E}_{(e, r, e_p) \in T} \left[ - \log \left( \frac{\exp(f(e, r, e_p))}{\sum_i \exp(f(e, r, e_i))} \right) \right],
\]

\[
\mathcal{L}_{\text{nonneg}}(T) = \mathbb{E}_{(e, r, e_p) \in T} \left[ - f(e, r, e_p) \right] + g(E),
\]

where \(T\) is the triple set of \(G\) and \(g(E)\) is a regularization function.

The two approaches have respective drawbacks. The former approach uses all entities except the target one as negative instances. It can provide a stable gradient for each epoch, while dramatically increasing computational complexity. In the latter approach, training positive triples only can minimize computation but tends to sink the model into a trivial optimum. Although previous work proposed some modifications to mitigate negative effects, they can only be applied to certain scoring functions and usually limit the prediction accuracy of KGE models.

Therefore, we argue that the feasible strategy replacing Negative Sampling should be somewhere between the two extreme approaches. We first combine the two training strategies to overcome their flaws. For all training triples in \(T\), we sample a small subset of triples \(\hat{T}\) to conduct the All-Negative training, while training the rest triples via the Non-Negative approach. Based on Eq. 2 and Eq. 3, we can re-organize the combined loss function as:

\[
\mathcal{L} = \mathcal{L}_{\text{allneg}}(\hat{T}) + \mathcal{L}_{\text{nonneg}}(T - \hat{T})
\]

\[
= \mathbb{E}_{(e, r, e_p) \in \hat{T}} \left[ - f(e, r, e_p) \right] + \mathbb{E}_{(e, r, e_p) \in T - \hat{T}} \left[ - \log \left( \frac{\exp(f(e, r, e_p))}{\sum_i \exp(f(e, r, e_i))} \right) \right]
\]

\[
= \mathbb{E}_{(e, r, e_p) \in \hat{T}} \left[ - f(e, r, e_p) \right] + \mathbb{E}_{(e, r, e_p) \in T - \hat{T}} \left[ \log \sum_i \exp(f(e, r, e_i)) \right]
\]

\[
= \frac{1}{n_T} \sum_{i=1}^{T} f(e, r, e_p) + \frac{1}{n_{\hat{T}}} \sum_{i=\hat{T}}^{T} \text{LSE}(f(e, r, E)),
\]

where the number of sampled triples \(n_{\hat{T}} = an_T\) and the hyper-parameter \(a \in [0, 1]\) determines the sampling proportion. \(\text{LSE}(\cdot)\) is the LogSumExp function, and the regularization part in \(\mathcal{L}_{\text{nonneg}}\) is omitted.

Drawing on the idea of Contrastive Learning, we can explain the intuitive sense of the reorganized loss function. From Eq. 4 we can see that the reorganized loss function contains two modules, which exactly satisfy two key properties of Contrastive Learning, Alignment and Uniformity. The first module is to achieve the Alignment property by maximizing the scores of all positive triples. In the vector space, this module maximizes the similarity of the query vector and its target vector in every pair. The second module minimizes the similarity of each sampled query vector with all entity vectors in \(G\). As all entity vectors are forced to stay away from these query vectors, the vector distribution tends to be uniform. Focusing on the two key properties, we propose a new query sampling loss for KGE models, which is defined as:

\[
\mathcal{L} = - \lambda \frac{1}{n_T} \sum_{i=1}^{T} f(e, r, e_p) + \frac{1}{n_{\hat{T}}} \sum_{i=\hat{T}}^{T} \text{LSE}(f(e, r, E)),
\]

where \(\lambda\) is a hyper-parameter to balance the contributions of two modules. As proved by a recent work in [27], learning both Alignment and Uniformity is a trade-off process. A completely uniform vector distribution makes alignment impossible, while aligning all positive pairs perfectly causes the clustered vectors indistinguishable. Therefore, the hyper-parameter \(\lambda\) is necessary to keep KGE training stable.
while All-Negative training is extremely redundant to separate all negative instances equally. As KGE training goes on, a large percentage of negative instances have been far away from the query vector, and thus provide less meaningful information. It would be more efficient if the loss can focus on negative instances that are difficult to be distinguished. To solve this issue, the contrastive loss in CL methods usually employs the temperature $\tau$. As shown in Eq. 1, the feature similarities are multiplied by $1/\tau$ before going through the Softmax function. As proved by the recent work [27], this temperature gives the contrastive loss a hardness-aware ability to control the strength of penalties on hard negative samples. However, in the All-Negative training condition, the number of negative instances could be much higher. Therefore, the distribution of the Softmax-normalized scores would be much more uniform, even using a higher temperature.

This problem guides us to review the recent low-dimensional hyperbolic-based KGE models [2, 5]. We find a key point overlooked in the past: the nonlinear function in the hyperbolic distance is beneficial to achieve the hardness-aware ability. There are two nonlinear functions utilized in previous low-dimensional KGE models, i.e., $h(x) = 2\text{Arctanh}(x) = \ln \frac{1+x}{1-x}$ and $h(x) = xe^x$. In Fig. 1, we can observe that their derivatives are always greater than one when $x \geq 0$. Besides, they have a similar trend as the value is relatively low at first and then increases rapidly. We argue that these nonlinear functions can be regarded as the activation function of KGE models. Given a KGE model with $\Psi(q,e) = ||q-e||_2^2$, the instance with higher $L_2$ distance is more likely to be negative. The nonlinear activation function can further amplify the distance value of an easy negative instance. Such that, the penalties of the indistinguishable negative instances would be strengthened in the loss.

Based on our observations, we design a Hardness-aware Activation mechanism to replace the hyperbolic geometry. As shown in Fig. 1, two existing nonlinear functions are upper unbounded, so they can only achieve a ‘soft constraint’ to negative instances. Some easy instances that have been successfully separated are still involved in gradient computing. There is a significant waste on large-scale KGs and it also negatively affects the alignment of the other triples. To this end, we attempt to add a ‘hard constraint’ by designing suitable upper-bounded activation functions. Referring to the existing nonlinear functions, we propose two novel hardness-aware activation functions, $\text{Hanon}(\cdot)$ and $\text{Halin}(\cdot)$, which are formulated as follows:

$$
\text{Hanon}(x) = \frac{1}{y^{-1} + e^{-\beta(x-0.5)}}
$$

(6)

$$
\text{Halin}(x) = \begin{cases} 
2x & 0 < x < 1 \\
\min(\beta(x - 1) + 2, y) & x \geq 1 
\end{cases}
$$

(7)

where $\beta$ and $y$ are the two hyper-parameters to control the soft and hard constraints. We set the soft-constraint parameter $\beta$ according to the slope of $h(x) = xe^x$. The curves of the two novel functions are shown in Fig. 1. The $\text{Hanon}(\cdot)$ can be regarded as a variant of the Sigmoid function but be upper bounded by $y$. The $\text{Halin}(\cdot)$ is a piecewise linear function. It has different slopes at the two sides of $x = 1$ and cuts the gradients when the value is more than $y$. It is clear that $\text{Hanon}(\cdot)$ and $\text{Halin}(\cdot)$ have similar slopes to the two previous functions when $x \leq y$. Then our functions use the ‘hard-constraint’ to cut the gradients of the distinguishable instances whose distance is bigger than $y$. We further improve the Hardness-aware Activation by multiplying the similarity score with a relation-specific trainable parameter. Applied by previous low-dimensional KGE models, this technology is beneficial to encoding hierarchical relationships and improves prediction accuracy [28]. Finally, given a query $(e, r)$ and its target entity $e_p$, the triple score based on $L_2$ distance via the Hardness-aware Activation is defined as:

$$
fh_a(e, r, e_p) = -h(\mathbf{e}_r \cdot \|\Phi(e, r) - e_p\|_2^2),
$$

(8)

where $h(\cdot)$ denotes the activation function $\text{Hanon}(\cdot)$ or $\text{Halin}(\cdot)$, and $\mathbf{e}_r$ is the relation-specific scalar parameter.
3.3 The HaLE Framework

To achieve swift and sure KGE training, the HaLE framework utilizes the Query Sampling loss to keep training stable and the Hardness-aware Activation mechanism to accelerate model convergence.

To integrate the two key techniques better, we apply the hardness-aware activation to two parts of our loss function in an asymmetric way. Specifically, we square the activated scores of positive instances in the Alignment part. Such that, the positive instances would get much stricter regularization than negative ones. The negative-activated instances would get bigger gradients than negative instances, and a positive instance whose $L_2$ distance is close to zero would make less contribution to the loss. We find that it can accelerate the model convergence further. Therefore, the final loss function of the HaLE framework is formulated as follows:

$$
\mathcal{L}_\text{HaLE} = -\lambda \frac{1}{n_T} \sum_{(e, r, e_p) \in T} \rho_{ha}(e, r, e_p) + \frac{1}{n_T} \sum_{(e, r, E) \in T} \mathcal{L}_{SE}(f_{ha}(e, r, E)),
$$

To verify the performance of our HaLE framework, we select five representative KGE models: TransE [3], DistMult [34], RotatE [22], RotE [5], and RotL [28]. These models utilize five different transform functions to generate the query vector in the Euclidean space, which are formulated as follows:

$$
\text{TransE}: \Phi_T(e, r) = e + r, \\
\text{DistMult}: \Phi_D(e, r) = e + r, \\
\text{RotatE}: \Phi_R(e, r) = \text{Rot}(e, r), \\
\text{RotE}: \Phi_E(e, r) = \text{Rot}(e, r)^T + r', \\
\text{RotL}: \Phi_L(e, r) = \text{Rot}(e, r) \odot r',
$$

where $\text{Rot}(\cdot)$ denotes the vector rotation operation, $r$ and $r'$ are two different relation vectors corresponding to the same relation $r$. To make a fair comparison, we use the $L_2$-distance squared similarity function $\Psi(q, e) = ||q - e||_2^2$. Although some previous works use the dot product function with specific regularization items, it has been proven to be equivalent to $L_2$ distance squared [36].

Compared with the previous Negative Sampling, All-Negative, and Non-Negative approaches, our HaLE framework can achieve sure and swift KGE training for several reasons:

- **The training process in one epoch is greatly accelerated.** The negative sampling for each triple is omitted, and the query sampling can significantly reduce the All-Negative training cost.
- **HaLE can provide a stable training target.** In each step of parameter optimization, we compute the gradients of all positive triples and force all entity vectors to stay away from the same part of queries.
- **The total training time is reduced.** The new loss can avoid parameter fluctuation, and the hardness-aware activation can focus on difficult instances. As a result, the HaLE-trained model can converge quickly in several epochs.

4 EXPERIMENTS

4.1 Experimental Setup

To verify the performance of HaLE, we focus on the link prediction, the most typical and challenging task for KG embeddings. Different from previous KGE research efforts that pursuing a higher prediction accuracy, we concentrate on the training efficiency of KGE models, which is critical for them to be applied in practice.

To compare the training efficiency of different strategies, we employ five representative KGE models as mentioned in Sec. 3.3 and train them in the specific space and time conditions. For the space condition, we set the dimension number of the low-dimensional models as 32 and high-dimensional ones as 256. For the time condition, we set a maximum training time according to the KG size of each dataset, as shown in Table 2. Following the previous work [3], we adopt two kinds of evaluation metrics in the ‘Filter’ mode: (1) MRR, the average inverse rank of the test triples, and (2) Hits@N, the proportion of correct entities ranked in top N. Higher MRR and Hits@N mean better performance.

4.1.1 Datasets. Our experimental studies are conducted on five commonly used datasets. WN18RR [4] is a subset of the English lexical database WordNet. FB15k237 [24] is extracted from Freebase including knowledge facts about movies, actors, awards, and sports. Compared with the FB15k dataset, it removes inverse relations because many test triples can be obtained simply by inverting triples in the training set. CoDEx-S/M/L [18] are three KG datasets with different scales extracted from Wikidata and Wikipedia. We only use positive triples in each dataset for a fair comparison. The statistics of the datasets are given in Table 2. ‘Train’, ‘Valid’, and ‘Test’ refer to the number of triples in the training, validation, and test sets.

4.1.2 Comparing Methods. We compare different training strategies mentioned in Sec. 3, including Negative Sampling (NS) [5], Self-Adversarial Negative Sampling (SaNS) [22], All-negative Training (All-Neg) [10] and Non-negative Training (Non-Neg) [14]. NS and SaNS utilize the binary cross entropy loss, while All-Neg utilizes the cross-entropy loss to compute all candidate entities. We implement a general Non-Neg strategy which uses a square loss to maximize positive triple scores and a global regularization to constrain the distance between each entity vector and the center vector of entity matrix. In the HaLE framework, we use the activation function

| Dataset     | nR | nE | #Train | #Valid | #Test | Time |
|-------------|----|----|--------|--------|-------|------|
| FB15k237    | 237| 14,541| 272,115| 17,535 | 20,466 | 1,200s |
| WN18RR      | 11 | 40,943| 86,845  | 3,034  | 3,134  | 600s  |
| CoDEx-S     | 42 | 2,034 | 32,888  | 1,827  | 1,828  | 300s  |
| CoDEx-M     | 51 | 17,050| 185,584 | 10,310 | 10,311 | 1,200s |
| CoDEx-L     | 69 | 77,951| 551,193 | 30,622 | 30,622 | 1,200s |
Table 3: Low-dimensional link prediction results on the WN18RR and FB15k237 datasets. The symbol ‘∗’ means the model is fully-trained, otherwise the model is trained in limited time. The best score of fully-trained models underlined and the best score of limited-trained models in Bold.

| Type               | Methods     | FB15k237 (1,200s) |            | WN18RR (600s) |            |
|--------------------|-------------|-------------------|------------|---------------|------------|
|                    |             | MRR      | Hits@10  | Hits@1        | MRR       | Hits@10  | Hits@1        |
| Hyperbolic-based   | MuRE [5]∗   | 0.323    | 0.501    | 0.235         | 0.465     | 0.544    | 0.420         |
| Models             | RotH [5]∗   | 0.312    | 0.489    | 0.224         | 0.447     | 0.518    | 0.408         |
|                    | RotH [5]∗   | 0.314    | 0.497    | 0.223         | 0.472     | 0.553    | 0.428         |
|                    | AttH [5]∗   | 0.324    | 0.501    | 0.236         | 0.466     | 0.551    | 0.419         |
| Negative Sampling  | TransE [3]  | 0.243    | 0.422    | 0.154         | 0.177     | 0.417    | 0.045         |
| Trained            | DistMult [34]| 0.278    | 0.445    | 0.194         | 0.351     | 0.482    | 0.283         |
|                    | RotatE [22]| 0.223    | 0.391    | 0.141         | 0.346     | 0.460    | 0.285         |
|                    | RotE [5]    | 0.246    | 0.424    | 0.159         | 0.355     | 0.480    | 0.290         |
|                    | RoL [28]    | 0.140    | 0.266    | 0.079         | 0.295     | 0.368    | 0.254         |
| HaLE Trained       | TransE [3]  | 0.314    | 0.492    | 0.224         | 0.212     | 0.492    | 0.028         |
|                    | DistMult [34]| 0.308    | 0.483    | 0.222         | 0.447     | 0.533    | 0.399         |
|                    | RotatE [22]| 0.307    | 0.479    | 0.219         | 0.451     | 0.536    | 0.406         |
|                    | RotE [5]    | 0.313    | 0.486    | 0.226         | 0.460     | 0.542    | 0.416         |
|                    | RoL [28]    | 0.516    | 0.493    | 0.228         | 0.471     | 0.558    | 0.424         |

Hanons ( ) by default. We also compare multiple activation functions shown in the Fig. 1.

4.1.3 Implementation Details. We select the hyper-parameters of our model via grid search according to the metrics on the validation set. For previous strategies, we select the learning rate among {0.0005, 0.001, 0.005}, the number of negative samples among {50, 256, 512}, the batch size among {256, 512, 1, 024}. For the HaLE framework, we select the sampling proportion \( \alpha \) among {0.05, 0.1, 0.2}, the balancing ratio \( \lambda \) among {0.1, 0.3, 0.5, 1.0}, the hard-constraint parameter \( \gamma \) among {5, 10, 20}. All experiments are performed on Intel Core i7–7700K CPU @ 4.20GHz and NVIDIA GeForce GTX1070 GPU, and are implemented in Python using the PyTorch framework.

4.2 Experimental Results

As Negative Sampling is the most commonly used training strategy in the KGE domain, we first compare the limited-time performance of different KGE models trained by Negative Sampling and HaLE (with Hanon). The 32-dimensional results on WN18RR and FB15k237 are shown in Table 3, while 256-dimensional results on three CoDEx datasets are shown in Table 4. Due to space constraint, the other experimental results including the ablation experiments and the visualization of entity embeddings can be found in Appendix.

4.2.1 Low-dimensional Performance Comparison. From Table 3, we have the following observations. Setting the limited training time as 1,200s for FB15k237 and 600s for WN18RR, the five different models trained by HaLE significantly outperform the NS-trained ones on both datasets. The MRR and Hits@10 of all models have an average 5% increase. The results indicate the effectiveness of the HaLE framework. In the five models, the HaLE-trained RoL model achieves the best performance in all metrics on two datasets, HaLE-RotE is the second. It proves the effectiveness of the rotation-translation form in the transform function. In addition, we find that the NS-trained RotL model is weaker than others. This is because the effect of the flexible addition operation relies on the nonlinear activation, which does not exist in the normal \( L_2 \)-distance similarity function. Compared with recent hyperbolic-based models, the simplest TransE model achieves competitive performance on FB15k237 after being trained in less than 20 minutes by HaLE. The HaLE-trained RotL model obtains the state-of-the-art MRR and Hits@10 on WN18RR, which has no hyperbolic geometry and only costs less than 10 minutes. It proves that the HaLE framework can make the Euclidean-base models to achieve high performance in low-dimensional conditions.

4.2.2 High-dimensional Performance Comparison. In the high-dimensional condition, HaLE shows a significant advantage over Negative Sampling. In the limited training time, HaLE can accelerate model convergence while NS-trained models fail due to the unstable gradients. This difference is more significant in the large-scale KGs. On the CoDEx-L dataset, the performance of TransE trained by HaLE is almost twice that of NS-trained TransE. Table 4 also lists the results of five fully-trained KGE models using more than 256 dimensions, which are detailed-tuned by a powerful hyperparameter optimization method [18]. Compared with them, the HaLE-trained models show strong competitiveness. Especially on CoDEx-M, the limited-time performance of the HaLE-TransE model outperforms that of the 512-dimensional TransE model. Although the Hits@1 of the optimal HaLE-RotL model is still lower than those benchmarks on CoDEx-L, HaLE-RotL achieves great Hits@10 results using less training time and fewer parameters. To sum up, training in a limited time, HaLE-trained models already obtain similar performance to the state-of-the-art models on five datasets. These results prove the efficiency of our HaLE framework on keeping high prediction accuracy.

4.2.3 Efficiency Comparison for Query Sampling. To verify the training efficiency of HaLE, we select the 32-dimensional RotE model and compare Query Sampling loss with four previous training strategies: NS, SaNS, All-Neg, and Non-Neg. The performance...


Table 4: High-dimensional link prediction results on the CoDEx datasets. The symbol ‘∗’ means the model is fully-trained, otherwise the model is trained in limited time. The best score of fully-trained models underlined and the best score of limited-trained models in Bold.

| Methods         | CoDEx-S (300s) | CoDEx-M (1,200s) | CoDEx-L (1,200s) |
|-----------------|---------------|-----------------|-----------------|
|                 | MRR Hits@10 Hits@1 | MRR Hits@10 Hits@1 | MRR Hits@10 Hits@1 |
| RESCAL [13]∗    | 0.404 0.623 0.293 | 0.317 0.456 0.244 | 0.304 0.419 0.242 |
| TransE [3]∗     | 0.354 0.634 0.219 | 0.303 0.454 0.223 | 0.187 0.317 0.116 |
| ComplEx [25]∗   | 0.465 0.646 0.372 | 0.337 0.476 0.262 | 0.294 0.400 0.237 |
| ConvE [7]∗      | 0.444 0.635 0.343 | 0.318 0.464 0.239 | 0.303 0.420 0.240 |
| TuckER [1]∗     | 0.444 0.638 0.339 | 0.328 0.458 0.259 | 0.309 0.430 0.244 |
| NS-TransE [3]   | 0.301 0.544 0.177 | 0.178 0.327 0.107 | 0.144 0.260 0.086 |
| NS-DistMult [34]| 0.360 0.589 0.246 | 0.255 0.395 0.182 | 0.228 0.353 0.164 |
| NS-RotaTE [22]  | 0.327 0.546 0.214 | 0.182 0.327 0.110 | 0.159 0.281 0.099 |
| NS-RotE [5]     | 0.328 0.549 0.214 | 0.183 0.330 0.112 | 0.155 0.270 0.097 |
| NS-RotL [28]    | 0.313 0.534 0.205 | 0.162 0.259 0.106 | 0.055 0.113 0.026 |
| HaLE-TransE [3] | 0.355 0.620 0.223 | 0.313 0.467 0.230 | 0.300 0.436 0.226 |
| HaLE-DistMult [34]| 0.403 0.629 0.289 | 0.314 0.462 0.236 | 0.299 0.427 0.230 |
| HaLE-RotaTE [22]| 0.407 0.635 0.289 | 0.324 0.474 0.244 | 0.302 0.435 0.229 |
| HaLE-RotE [5]   | 0.409 0.659 0.291 | 0.326 0.475 0.246 | 0.308 0.438 0.257 |
| HaLE-RotL [28]  | 0.408 0.659 0.292 | 0.324 0.474 0.244 | 0.308 0.438 0.238 |

5 RELATED WORK

Recently, knowledge graph completion via KGE has been an active research topic [30]. Dozens of KGE models have been proposed, which can be divided into three categories from the perspective of the scoring function: (1) geometric distance based models, including TransE [3], TransD [9], RotaTE [22], QuaTE [35]; (2) tensor factorization based models, including RESCAL [13], DistMult [34], ComplEx [25], TuckER [1]; and (3) deep learning based models, including ConvE [7], ConvKB [12], RGCN [21], CompGCN [26]. All current KGE models suffer from the same issues of low speed and high cost in the training phase. The problem become much more serious when processing large-scale KGs with millions or billions of entities. Recently, several researchers have worked on this issue via different technical channels.

Reducing Parameters. Limiting the vector dimensions as 32 or 64, several low-dimensional KGE models are proposed to achieve competitive performance with less trainable parameters. MuRP [2] is the first KGE model based on hyperbolic vector space, and outperforms previous models in the low-dimensional condition. It embeds KG triples in the Poincaré ball model using the Möbius matrix-vector multiplication and Möbius addition operations. To further capture logical patterns in KGs, Chami et al. [5] propose a series of hyperbolic KGE models, including RotH, RefH, and AtiH. These models utilize vector rotation or reflection operations.

changes of the validation set as training proceeds are shown in the three upper line charts in Fig. 2. It is clear that our HaLE achieves remarkable efficiency on the three datasets comparing with the previous strategies. Besides, there are some common observations in the three results. Except Non-Neg, the negative sampling is the worst one whose Hits@10 slowly increases in the first 50 seconds, indicating the negative effect of unstable gradients. Assigning different weights to negative instances, SaNS has a much faster convergence speed than NS. Outperforming NS and SaNS, the All-Neg strategy has good performance on two large datasets FB15k237 and CoDEx-M. As the WN18RR is relatively sparse, All-Neg is slightly inefficient to train all negative instances using a uniform gradient. These results prove the effectiveness of the All-Negative training and hardness-aware ability. Without negative instances, the Non-Neg strategy is the only unstable one. Keeping increasing in the first 80 seconds, the Hits@10 of Non-Neg starts decreasing, because its negative constraint is not powerful enough to avoid over-fitting. Our HaLE achieves the fastest convergence speed on the three datasets. Especially on WN18RR, HaLE achieves more than 0.5 Hits@10 in the first 30 seconds, which is already better than the final results of the others, indicating that HaLE can achieve a swift and sure KGE training, and has considerable potential in practical applications.

4.2.4 Efficiency Comparison for Hardness-aware Activation. To verify the hardness-aware activation and our novel activation functions, we compare the performance of different activation functions in the HaLE framework. The results are shown in the three lower line charts in Fig. 2. We can find similar observations on the three datasets. At first, utilized in hyperbolic models, the Arctanh-based function is obviously weaker than others. As its definition range is (−1, 1), it relies on the normalization effect of hyperbolic geometry. In the two linear functions, the 𝑦 = 2𝑥 function is simulating the temperature control in CL methods and our Halin(·) can be regarded as an extended version of the former with soft- and hard-constraints. It is clear that the Hits@10 of 𝑦 = 2𝑥 increases faster in the first few rounds but gets a lower final Hits@10. Then We can see that the performance of Hanon(·), Halin(·) and 𝑦 = xe𝑥 are very close. On the CoDEx-M and WN18RR datasets, our Hanon function performs the best. It is because Hanon has an additional hard-constraint property to limit the outputted maximum. The 𝑦 = xe𝑥 function used in the original RotL model is slightly better than Hanon(·) in FB15k237. The linear function Halin(·) achieves similar performance with the two nonlinear ones, proving that the soft- and hard-constraints are the key properties of the hardness-aware activation.
to replace the multiplication operation between the head entity and relation vectors. Based on the RotH model, Wang et al. [28] propose two Euclidean-based lightweight models, RotL and Rot2L. Eliminating complex hyperbolic operations, the two models have lower computational complexity and faster convergence speed.

Replacing Negative Sampling. Most current KGE models are trained via negative sampling, which considers only a subset of negative instances to reduce the time complexity of each training epoch. However, negative sampling usually extends the convergence time of KGE models because of additional sampling calculations and unsteady training gradients. To solve this issue, Li et al. [10] propose an efficient All-Negative training framework and reduce the complexity of All-Negative calculations by dis-entangling the interactions between entities. However, this framework can only be applied to KGE models using a square-based loss. Its accuracy is lower than models trained by the negative sampling loss, especially in the low-dimensional condition. Peng et al. [14] employ segmented embeddings for parallel processing, and propose a Non-Negative strategy utilizing two vector constraints to replace negative sampling. However, these techniques cause a decrease in accuracy and force the model to use higher-dimensional vectors to represent each entity (e.g., 2,000 dimensions in [14]). Besides, this framework is based on Orthogonal Procrustes Analysis, and cannot be applied to existing KGE models directly.

Accelerating Model Convergence. Some recent research efforts design new loss functions to accelerate the convergence of KGE models. Sun et al. [22] propose a self-adversarial negative sampling technique for efficiently and effectively training the RotatE model. It can be regarded as an improved binary cross-entropy loss, treating the normalized triple score as the weight of each negative sample. Another way is adding soft label loss based on the knowledge distillation technique. DistilE [38] utilizes an additional soft-label loss based on the knowledge distillation technique. A pre-trained high-dimensional KGE model generates soft labels for each training sample and accelerates the convergence of the small student model. MulDE [29] is a multi-teacher knowledge distillation framework for KGE models. Instead of a high-dimensional model, MulDE employs multiple low-dimensional models as teachers jointly supervising the student model via a novel iterative distillation strategy. Although the knowledge distillation framework can train a student KGE model quickly, it still requires the pre-training of teacher models and cannot really reduce training cost.

On top of the above research work, there are some well-engineered systems for accelerating KGE training, such as OpenKE [8] and DGL-KE [37]. To make full use of hardware computation power, these systems convert KGE models to multi-thread versions or deploy them in distributed parallel hardware. In this paper, we focus on the algorithmic improvement of KGE models.

6 CONCLUSION

Recent knowledge graph embedding (KGE) models excessively pursue prediction accuracy but ignore the training efficiency. In this paper, we propose a novel Hardness-aware Low-dimensional Embedding (HaLE) framework to achieve a swift and sure KGE training. Motivated by the newest findings in the Contrastive Learning domain, we propose two key techniques: Query Sampling Loss and Hardness-aware Activation. We describe the connections of the two techniques with previous KGE achievements and prove
their effectiveness by comparing with four previous training strategies in the link prediction task. The experimental results show that HaLE can achieve both higher prediction accuracy and faster convergence speed in limited training time.

These positive results encourage us to explore further research activities in the future. Instead of using artificially designed activation functions, we will apply the Neural Architecture Search technology to find more powerful activation functions automatically. Facing large-scale KGs, All-Negative training is still a burden. We aim to filter out some negative instances before measuring scores based on the hard-constraint mechanism. Finally, we will apply HaLE to other KG tasks, such as KG alignment and triple classification, to further verify the performance of the proposed framework.

REFERENCES

[1] Ivana Balazevic, Carl Allen, and Timothy Hospedales. 2019. TuckER: Tensor Factorization for Knowledge Graph Completion. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th Joint Conference on Natural Language Processing (EMNLP-JCNLP). Hong Kong, China, 5185–5194.

[2] Ivana Balazevic, Carl Allen, and Timothy M. Hospedales. 2019. Multi-relational Poincaré Graph Embeddings. In Proceedings of the 33rd Annual Conference on Neural Information Processing Systems, NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada. 4465–4475.

[3] Antoine Bordes, Alberto García-Durán, Jason Weston, and Oksana Yakhnenko. 2013. Translating Embeddings for Modeling Multi-relational Data. In Proceedings of the 29th Conference on Neural Information Processing Systems, December 5-8, 2013, Lake Tahoe, Nevada, United States. 2787–2795.

[4] Antoine Bordes, Xavier Glorot, Jason Weston, and Yosua Bengio. 2014. A Semantic Matching Energy Function for Learning with Multi-relational Data. The Journal of Machine Learning Research 14 (2014), 235–259.

[5] Ines Chami, Adva Wolf, Da-Cheng Juan, Frederic Sala, Sujith Ravi, and Christopher Ré. 2020. Low-Dimensional Hyperbolic Knowledge Graph Embeddings. In Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics, ACL 2020, Online, July 5-10, 2020. 6901–6914.

[6] Ting Chen, Simon Kornblith, Mohammad Norouzi, and Geoffrey E. Hinton. 2020. A Simple Framework for Contrastive Learning of Visual Representations. In Proceedings of the 37th International Conference on Machine Learning, ICML 2020, 13-18 July 2020, Virtual Event. 1597–1607.

[7] Tim Dettmers, Pasquale Minervini, Pontus Stenetorp, and Sebastian Riedel. 2018. Convolutional 2D Knowledge Graph Embeddings. In Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence, AAAI-18, New Orleans, Louisiana, USA, February 2-7, 2018. 1811–1818.

[8] Xu Han, Shulin Cao, Xin Ly, Yanlinkai Liu, Zhiyuan Liu, Maosong Sun, and Jianzhi Li. 2018. OpenKE: An Open Toolkit for Knowledge Embedding. In Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing, EMNLP 2018, System Demonstrations, Brussels, Belgium, October 31 - November 4, 2018. 139–144.

[9] Guoliang Ji, Shixiu He, Lihe Xing, Kang Liu, and Jun Zhao. 2015. Knowledge Graph Embedding via Dynamic Mapping Matrix. In Proceedings of the 33rd Annual Meeting of the Association for Computational Linguistics and the 7th International Joint Conference on Natural Language Processing (Volume 1: Long Papers). Beijing, China, 687–696.

[10] Zelong Li, Jianchao Ji, Zuohui Fu, Guanyi Chen, Chenghua Lin, and Mark Stevenson. 2021. Highly Efficient Knowledge Graph Embedding Learning with Orthogonal Procrustes Analysis. In Proceedings of the 2021 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, NAACL-HLT 2021, Online, June 6-11, 2021. 2364–2375.

[11] Paolo Rosso, Dingyi Yang, Natalia Ostapuk, and Philippe Cédrit-Mauroux. 2020. BETA: A Schema-Matching-Based End-to-End Solution for Instance Completion in Knowledge Graphs. In Proceedings of the WWW ’21: The Web Conference 2021, Virtual Event / Ljubljana, Slovenia, April 19-23, 2021. 845–856.

[12] Daniel Ruffinelli, Samuel Broschert, and Rainer Gemulla. 2020. You CAN Teach an Old Dog New Tricks! On Training Knowledge Graph Embeddings. In Proceedings of the 8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020.

[13] Maximilian Nickel, Volker Tresp, and Hans-Peter Kriegel. 2011. A Three-Way Model for Collective Learning on Multi-Relational Data. In Proceedings of the 28th International Conference on Machine Learning, ICML 2011, Bellevue, Washington, USA, June 28 - July 2, 2011. 809–816.

[14] Xutan Peng, Guanyi Chen, Chenghua Lin, and Mark Stevenson. 2021. Highly Efficient Knowledge Graph Embedding Learning with Orthogonal Procrustes Analysis. In Proceedings of the 2021 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, NAACL-HLT. 1, 2021. 2364–2375.

[15] Tim Dettmers, Pasquale Minervini, Pontus Stenetorp, and Sebastian Riedel. 2015. Compositional Models for Knowledge Graphs. In Proceedings of the 5th Workshop on Graph Representation Learning, 2015. 1727–1736.
[34] Bishan Yang, Wen-tao Yih, Xiaodong He, Jianfeng Gao, and Li Deng. 2015. Embedding Entities and Relations for Learning and Inference in Knowledge Bases. In Proceedings of the 3rd International Conference on Learning Representations, ICLR 2015, San Diego, CA, USA, May 7-9, 2015.

[35] Shuai Zhang, Yi Tay, Lina Yao, and Qi Liu. 2019. Quaternion Knowledge Graph Embeddings. In Proceedings of the Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada. 2731–2741.

[36] Zhanqiu Zhang, Jianyu Cai, and Jie Wang. 2020. Duality-Induced Regularizer for Tensor Factorization Based Knowledge Graph Completion. In Proceedings of the 34th Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual.

[37] Da Zheng, Xiang Song, Chao Ma, Zeyuan Tan, Zihao Ye, Jin Dong, Hao Xiong, Zheng Zhang, and George Karypis. 2020. DGL-KE: Training Knowledge Graph Embeddings at Scale. In Proceedings of the 43rd International ACM SIGIR conference on research and development in Information Retrieval, SIGIR 2020, Virtual Event, China, July 25-30, 2020. 739–748.

[38] Yushan Zhu, Wen Zhang, Hui Chen, Xu Cheng, Wei Zhang, and Huajun Chen. 2020. DistilE: Distilling Knowledge Graph Embeddings for Faster and Cheaper Reasoning. CoRR abs/2009.05912 (2020). https://arxiv.org/abs/2009.05912