Abstract

Link prediction plays an important role in knowledge graph domain. According to the literature survey [Wang et al., 2017], knowledge graph embedding methods can be classified into translational distance models and semantic matching models.

The translation distance model uses the distance-based scoring function to express the different relationships between nodes by designing the distance evaluation method of different nodes. TransE [Bordes et al., 2013] and TransH [Wang et al., 2014] were proposed to model relationships by interpreting them as translations operating on the low-dimensional embeddings of the entities. RotatE [Sun et al., 2018], which defines each relation as a rotation from the source entity to the target entity in the complex vector space, is able to model and infer various relation patterns including: symmetry/antisymmetry, inversion, and composition. HAKE [Zhang et al., 2020c] combined TransE and RotatE to model entities at different levels of a hierarchy while distinguishing entities at the same level in a hierarchy. GAAT [Wang et al., 2019] introduced Graph Attenuated Attention structure to integrate an attenuated attention mechanism to assign different weight in different relation path and acquire the information from the neighborhoods. Although the distance representation of entity relations based on translation distance representation is very diverse, it is difficult to predict the entity information that has not appeared.

Method based on semantic matching models is not affected by cold start, and better representations can be obtained for unseen entities based on text information. KG-BERT [Yao et al., 2019], a novel framework named Knowledge Graph Bidirectional Encoder Representations from Transformer, was presented with treating triples in knowledge graphs as textual sequences. MLMLM [Clouatre et al., 2020] established a mapping from language model to knowledge base by comparing the mean likelihood of generating the different entities to perform link prediction in a tractable manner. StAR [Wang et al., 2021] partitioned each triple into two asymmetric parts as in translation-based graph embedding approach, and encode both parts into contextualized representations by a Siamese-style textual encoder. However, the pre-training stage of textual models only learned the context knowledge of the text, but ignored the relationship information. Moreover, the model structure is usually complex, and it is difficult to do a high proportion of negative sampling, resulting in insufficient learning of negative sample information in the training process, which limits the effect of the model.

In this study, aiming to solve the problem of poor prediction of the unseen node of the translation distance model and insufficient training of the text matching model, we propose a new knowledge graph BERT pre-training framework, named LP-BERT. LP-BERT, which is a semantic matching representation model, uses a multi-task pre-training strategy, which not only uses MLM to learn the knowledge of context corpus, but also introduces entity semantic prediction and relational...
semantic prediction tasks to learn the relationship information of triples. It allows structured knowledge graph relational information to be learned in the pretraining phase as unstructured semantic knowledge. Moreover, inspired by contrastive learning, we carry out a triple-style negative sampling in sample batch, which greatly increased the proportion of negative sampling while ensuring that the training time remains unchanged, to solve the problem of insufficient model training caused by the low negative sampling ratio. At the same time, we propose a data augmentation method based on the inverse relationship of triples to further increase the sample diversity.

We comprehensively evaluate the performance of LP-BERT using WN18RR, FB15k-237 and UMLS datasets. Without bells and whistles, LP-BERT outperforms related work [Song et al., 2021; Gao et al., 2021; Peng and Zhang, 2020; Zhang et al., 2020c; Wang et al., 2021] and achieve state-of-the-art results on WN18RR and UMLS datasets, especially the Hits@10 indicator improved by 5% from the previous state-of-the-art result on WN18RR dataset and achieve 100% Hits@10 on UMLS dataset.

2 Related Work

2.1 Link Prediction

Link prediction is an important research area in knowledge graph embedding and received a lot of attention in recent years. KBGAT [Nathani et al., 2019], a novel attention based feature embedding, was proposed to capture both entity and relation features in any given entity’s neighborhood. AutoSF [Zhang et al., 2020a] is a method automatically design SFs for distinct KGs by the AutoML techniques. CompGCN [Vashishth et al., 2019] is a novel Graph Convolutional framework which jointly embeds both nodes and relations in a relational graph, which leverages a variety of entity-relation composition operations from Knowledge Graph Embedding techniques and scales with the number of relations. MetaKGR [Lv et al., 2019] is a meta-based multi-hop reasoning method, which adopts meta-learning to learn effective meta parameters from high-frequency relations that could quickly adapt to few-shot relations. CompEx-N3-RP [Chen et al., 2021] is a new self-supervised training objective for multi-relational graph representation learning, via simply incorporating relation prediction into the commonly used 1vsAll objective, which contains not only terms for predicting the subject and object of a given triple, but also a term for predicting the relation type. Atth [Chami et al., 2020] is a class of hyperbolic KG embedding models that simultaneously capture hierarchical and logical patterns, which combines hyperbolic reflections and rotations with attention to model complex relational patterns.

2.2 Language Model Pre-training

MLM-based pre-training method used in BERT [Devlin et al., 2018] opens up a pre-training paradigm of language model based on transformer structure. RoBERTa [Liu et al., 2020] carefully measures the impact of key hyperparameters and training data size and further enhance the effect. SpanBERT [Joshi et al., 2020] extends BERT by masking contiguous random spans, rather than random tokens, and training the span boundary representations to predict the entire content of the masked span, without relying on the individual token representations within it. MacBERT [Cui et al., 2020] improves upon RoBERTa in several ways, especially the masking strategy that adopts MLM as correction (Mac). In the field of knowledge graph, KG-BERT [Yao et al., 2019] uses the MLM method for pre-training on the triple data to learn the corpus information of the knowledge graph scene. Unlike these studies, we use a multi-task pre-training strategy based on MLM, Mask Entity Model (MEM) and Mask Relation Model (MRM), so that the model can not only learn context corpus information, but also learn the association information of triples at the semantic level.

3 LP-BERT

3.1 Overall Framework

The framework of our proposed LP-BERT is shown in Figure 1. The whole framework can be divided into two learning stages: multi-task pre-training stage and knowledge fine-tuning stage. Different from the traditional Mask Language Model (MLM)-based pre-training method, we propose a multi-task pre-training method which contains three tasks: MLM, Mask Entity Model (MEM) and Mask Relation Model (MRM) three tasks, so that LP-BERT can not only learn the context corpus information in the task scene, but also fully learn the relationship information of the head-relation-tail triple at the semantic level. In the knowledge fine-tuning stage, inspired by contrastive learning, we carry out a triple-style negative sampling in sample batch, which greatly increased the proportion of negative sampling while keeping the training time almost unchanged. Furthermore, we propose a data augmentation method based on the inverse relationship of triples to further increase the sample diversity. At the same time, mixed precision strategy is introduced to reduce the GPU memory and further improve the negative sampling ratio.

![Figure 1: An overview of the overall framework. Training process of LP-BERT contains pre-training and fine-tuning two phases. Pre-training phase is a multi-task training for triple text containing MEM, MRM, MLM three tasks. The fine-tuning stage encodes $E_h, R$ and $E_t$ respectively, using two different distances $Dis_1$ and $Dis_2$ to calculate the loss and update the model parameters respectively.](image)

3.2 Multi-task Pre-training

We propose a pre-training strategy based on MLM, MEM and MRM three tasks. We define $(E_h, R, E_t)$ to express triple,
For each triple sample, there are three possible approaches: MEM, MEM\_t and MRM. The predicted targets of the three tasks correspond to an element in the triad, respectively. The predicted targets of MEM\_t and MRM are \(X^{E_t}, X^{R_t}\) and \(R\), which are word sequences marked with different colors, respectively. Different tasks have different mask areas, represented by [MASK] flags with different colors. The MEM, MRM and MRM\_t losses are calculated separately and then merged together to update the gradient.

\(D_h\) and \(D_t\) represent the description features of \(E_h\) and \(E_t\) respectively. Specifically, a BERT tokenizer firstly transforms the text \(x\) of each entity/relation/description to a sequence word embeddings \(X = [x_1, ..., x_n] \in \mathbb{R}^{d \times n}\). So, the text of \(E_h\), \(R\), \(E_t\), \(D_h\) and \(D_t\) can be denoted as \(X^{(E_h)}\), \(X^{(R)}\), \(X^{(E_t)}\), \(X^{(D_h)}\) and \(X^{(D_t)}\). For each triple, we combine the whole text of the total elements as follows:

\[
\tilde{X} = [x^{[CLS]}, X^{(E_h, D_h)}, x^{[SEP]}, X^{(R)}, x^{[SEP]}, X^{(E_t, D_t)}, x^{[SEP]}]
\]

(1)

where [CLS] and [SEP] are special tokens defined in [Devlin et al., 2018]. \(\tilde{X}\) is the input features sequence of the model.

For different tasks, different mask strategies are used to process the samples. The sample processing for each task is described in detail below.

**Mask Entity Modeling (MEM)**

For semantic based entity prediction task, since each triple includes two entities: head entity and tail entity. We have defined two different tasks: head entity prediction and tail entity prediction. For tail entity prediction, we construct the features and prediction objectives of the sample as follows:

\[
\tilde{X} = [x^{[CLS]}, X^{(E_h, D_h)}, x^{[SEP]}, X^{(R, [MASK]), [PAD]}], x^{[SEP]}]
\]

(2)

\[
\tilde{Y} = [x^{[CLS]}, X^{([PAD])}, X^{(E_t, [PAD])}, x^{[SEP]}]
\]

(3)

where \(\tilde{X}\) and \(\tilde{Y}\) are the input features and prediction objectives for the tail entity prediction task, respectively; \(X^{([MASK])}\) is the [MASK] sequence of the \(E_t\), and the number of \(X^{([MASK])}\) is the same as the length of the word tokens sequence of \(E_t\) \(X^{(E_t)}\); \(X^{([PAD])}\) in \(\tilde{X}\) and \(\tilde{Y}\) are the sequences of [PAD] tokens to complement the entire sequence to a fixed length. The length of \(X^{([PAD])}\) in \(\tilde{Y}\) is the same as the sum of \(X^{(E_h, D_h)}\) and \(X^{(R)}\). \(X^{([PAD])}\) sequences are not involved in the calculation of the loss.

An EM-head \(y = BN(\text{GeLU}(\text{MLP}(X_{\text{encoded}})) + \text{bias})\), which combines a multilayer perceptron and batchnorm layer, is added after LP-BERT encoder to output the probability matrix of the prediction results. Each token has a probability vector of the word vocabulary size, but the prediction results are not involved in the loss calculation except the tokens of \(X^{(E_t)}\). Similarly, for the prediction of head entities, mirroring constructs text features and prediction objectives as follows:

\[
\tilde{X} = [x^{[CLS]}, X^{([MASK]), [PAD]}], X^{(R, E_t, D_t, [PAD])}, x^{[SEP]}]
\]

(4)

\[
\tilde{Y} = [x^{[CLS]}, X^{(E_h)}, X^{([PAD])}, x^{[SEP]}]
\]

(5)

where the length of \(X^{([MASK])}\) in \(\tilde{X}\) is the same as \(X^{(E_h)}\) in \(\tilde{Y}\), and the length of \(X^{([PAD])}\) in \(\tilde{Y}\) is the same as the sum of \(X^{(E_t)}\), \(X^{(D_h)}\) and \(X^{(R)}\) in \(\tilde{Y}\).

For the MEM task, the samples predict whether the head entity or the tail entity is random in the training process, and the two probabilities are the same.

**Mask Relation Modeling (MRM)**

For the relation prediction task, the sample construction strategy is similar to the MEM task. While preserving the head and tail entities and descriptions in the triple, the token sequence of the relation is masked and predicted. The characteristics and target construction of the sample are as follows:

\[
\tilde{X} = [x^{[CLS]}, X^{(E_h, D_h)}, x^{[SEP]}, X^{([MASK]), E_t, D_t}], x^{[SEP]}]
\]

(6)

\[
\tilde{Y} = [x^{[CLS]}, X^{([PAD])}, x^{[SEP]}, X^{(R, [PAD])}, x^{[SEP]}]
\]

(7)
Mask Language Modeling (MLM)
In order to coexist with MEM and MRM, unlike BERT's [Devlin et al., 2018] random masking prediction of all tokens in the sequence, the proposed MLM method only makes local random masking for the specific text range of the sample. The random masking strategy is as follows:
- For head entity prediction task in MEM, random mask only in token sequences of $E_t$ and $D_t$ ($X(E_t, D_t)$).
- For tail entity prediction task in MEM, random mask only in token sequences of $E_h$ and $D_h$ ($X(E_h, D_h)$).
- For MRM task, random mask only in token sequences of $E_h, D_h, E_t$ and $D_t$ ($X(E_h, D_h, E_t, D_t)$).

In this way, the model not only learns the context information of the corpus, but also does not affect label construction of MEM and MRM tasks. At the same time, doing masking is equivalent to doing dropout-like regularization for the text features of MEM and MRM tasks and it can improve the performance of MEM and MRM shown from experiments.

Pre-training Loss Designing
Since the strategies of constructing samples in MEM and MRM tasks are mutually exclusive, the prediction of head entity and tail entity cannot be simultaneously predicted for the triple samples trained by the same input model. To ensure the generalization ability of the model, we merge MEM and MRM tasks into Mask Item Model (MIM) task and define loss function as follows
\[
L = L_{MLM}(y', y) + L_{MIM}(y', y|\alpha) \tag{8}
\]
where $L$ is the final loss, $y'$ and $y$ are the prediction objectives and results, respectively, and $\alpha$ is the random number uniformly distributed in the interval $[0, 1]$. Details of $L_{MIM}$ shown as follows:
\[
L_{MIM}(y', y|\alpha) = \begin{cases} 
L_{MEM}(y', y) & 0.0 \leq \alpha < 0.4 \\
L_{MIM}(y', y) & 0.4 \leq \alpha < 0.8 \\
L_{MIM}(y', y) & 0.8 \leq \alpha < 1.0 
\end{cases} \tag{9}
\]

3.3 Knowledge Graph Fine-tuning

Knowledge Representation
The sample construction method in fine-tuning stage is different from that in pre-training stage. Inspired by the StAR [Wang et al., 2021], for the triple sample, we connect $E_h$ and $R$ texts. The pre-trained LP-BERT model uses the structure of siamese [Mueller and Thayagarajan, 2016] to encode $E_t, R$ and $E_r$ texts, respectively. The gradient update model parameters are calculated by making the positive vector pair closer and the negative vector pair further to fine-tune the model.

Contrastive Learning
Using the contrastive learning method, negative sampling is carried out in each sample batch, as shown in the Figure 3. For each sample in the batch, LP-BERT encodes the knowledge representation, and then calculates the distance in pairs. The size of batch is defined as $n$. Each entity element in batch has a positive case and $n - 1$ negative cases. Therefore, every batch the complex model LB-BERT only encodes $2n$ times, but actually does $n - 1$ times negative sampling and calculates $n^2$ sample distance, which greatly increases the proportion of negative sampling and reduces the training time.

![Figure 3: Label matrix in a batch. The batch size is $n$. For the $i$th($i \in n$) element in batch, composed of $E_h, R$, and $E_t$. For $E_h, R$, and $E_t$, they each participated in the composition of 1 positive sample and $n - 1$ negative samples. Therefore, there are $n^2$ samples in the batch, including $n$ positive samples and $n(n - 1)$ negative samples.](image)

\[
\text{Triple Augmentation}
\]

The $(E_h, R, E_t)$ pair-based knowledge graph representation method defined by StAR [Wang et al., 2021] has certain limitations. This method cannot represent $(E_h, RE_t)$ pair vectors directly in head entity prediction task. In particular, for the contrastive learning method that we use to conduct negative sampling in batch, can only make negative sampling for $E_t$, but cannot for $E_h$, which greatly limits the diversity of sampling. The more types of data set relationships are, the more obvious this disadvantage is. Therefore, we propose a dual inverse relationship data enhancement method. For each relationship $R$, we define a corresponding inverse relationship $R_{rev}$, or the head entity prediction sample in the form of (? , $R , E_r$), we rewrite it into the form of ($E_r , R_{rev} , ?$) to enhance the data. In this way, for the vector representation of $(E_h, RE_t)$ pairs, we can replace the vector representation of $(E_tR_{rev}, E_h)$ pairs, so that the knowledge map vector representation method for predicting head entity tasks is consistent with the tail entity prediction task, which greatly improves the diversity of sampling and the robustness of the model.

Mixed Precision
Moreover, we use the mixed precision strategy of fp16 and fp32 to reduce the GPU memory usage of gradient calculation to further improve the size of $n$ and increase the negative sampling ratio.

Fine-tuning Loss Designing
We designed two distance calculation methods to jointly calculate the loss function,
\[
L = L_1(V_{E_h, R}, V_{E_t}) + L_2(V_{E_h, R}, V_{E_t}) \tag{10}
\]
where $V_{E_h, R}$ and $V_{E_t}$ are encoded vectors of $E_h, R$ and $E_t$, respectively.

\[
L_1(d_1) = \begin{cases} 
-\alpha_t(d_1)^\gamma \log(d_1) & y = 1 \\
-\alpha_t(d_1)^\gamma \log(1 - d_1) & y \neq 1 
\end{cases} \tag{11}
\]
\[
L_2(d_2) = \begin{cases} 
\text{Sigmoid}(\text{sum}(d_2)) & y = 1 \\
1 - \text{Sigmoid}(\text{sum}(d_2)) & y \neq 1 
\end{cases} \tag{12}
\]
4 Experiments

This section is organized as follows. First, we introduce the experimental settings in detail. Then, we show the effectiveness of our proposed model on WN18RR [Dettmers et al., 2018] FB15k-237 [Toutanova et al., 2015] and UMLS [Dettmers et al., 2018] benchmark datasets. Finally, we show the results of ablation studies.

4.1 Experiment Settings and Datasets

We evaluate our proposed models on WN18RR [Dettmers et al., 2018], FB15k-237 [Toutanova et al., 2015] and UMLS [Dettmers et al., 2018] datasets. WN18RR is a link prediction dataset from WordNet [Miller, 1998]. It consists of English phrases and their semantic relations. FB15k-237 [Toutanova et al., 2015] is a subset of Freebase, consisting of real-world named entities and their relations. WN18RR and FB15k-237 are updated from WN18 and FB15k [Bordes et al., 2013] respectively by removing inverse relations and data leakage, which is the most popular benchmark. UMLS [Dettmers et al., 2018] is a small KG containing medical semantic entities and their relations. Summary stats are shown in Table 2

where

\[
\begin{align*}
    d_1 &= \frac{\langle v_{E_1}, v_{E_2} \rangle}{\|v_{E_1}\| \|v_{E_2}\|} \\
    d_2 &= \|v_{E_1} - v_{E_2}\| 
\end{align*}
\]

where \(\alpha\) is used to adjust the weights of positive and negative samples, \(\gamma\) is used to adjust the weights of samples that are difficult to distinguish. Two different dimensional distance calculation methods are used to calculate the distance relationship between multi-task learning vector pairs.

### Table 1: Results on WN18RR, FB15k-237 and UMLS datasets. Resulting numbers are taken from the original papers. The bold numbers denote the best results in each genre while the underlined ones are state-of-the-art performance. We can see that LP-BERT achieves SOTA in multiple evaluation results on WN18RR and UMLS datasets, and outperforms other semantic matching models on the FB15k-237 dataset.

| Methods          | WN18RR | FB15k-237 | UMLS |
|------------------|--------|-----------|------|
|                  | Hits@1 | Hits@3 | Hits@10 | MR   | MRR  | Hits@1 | Hits@3 | Hits@10 | MR   | MRR  | Hits@10 | MR   | MRR  |
| TransE [Bordes et al., 2013] | 0.403 0.441 0.532 | 2300 0.243 | 0.198 0.376 | 0.441 323 0.279 | 0.989 1.84 |
| DistMult [Yang et al., 2014] | 0.412 0.470 0.504 | 7000 0.444 | 0.199 0.301 | 0.446 512 0.281 | 0.846 5.52 |
| ComplEx [Trouillon et al., 2016] | 0.409 0.469 0.530 | 7882 0.449 | 0.194 0.297 | 0.450 546 0.278 | 0.967 2.59 |
| R-GCN [Schlichtkrull et al., 2018] | 0.080 0.137 0.207 | 6700 0.123 | 0.100 0.181 | 0.300 600 0.164 | - - |
| ConvE [Dettmers et al., 2018] | 0.419 0.470 0.531 | 4464 0.456 | 0.225 0.341 | 0.497 245 0.312 | 0.990 1.51 |
| KBAT [Nathani et al., 2019] | - - 0.554 | 1921 0.412 | - - 0.331 270 0.157 | - - |
| QuatE [ZHANG et al., 2019] | 0.436 0.500 0.564 | 3472 0.481 | 0.221 0.342 | 0.495 176 0.311 | - - |
| RotAE [Sun et al., 2018] | 0.428 0.492 0.571 | 3340 0.476 | 0.241 0.375 | 0.533 177 0.338 | - - |
| TuckER [Baláževič et al., 2019] | 0.443 0.482 0.526 | - - 0.470 | 0.266 0.394 | 0.544 - 0.358 | - - |
| AttH [Chami et al., 2020] | 0.443 0.499 0.573 | - - 0.486 | 0.252 0.384 | 0.540 - 0.348 | - - |
| ConE [Bai et al., 2021] | 0.453 0.515 0.579 | - - 0.496 | 0.247 0.381 | 0.54 - 0.345 | - - |
| DensE [Lu and Hu, 2020] | 0.443 0.508 0.579 | 1032 0.491 | 0.256 0.384 | 0.535 169 0.349 | - - |
| Rot-Pro [Song et al., 2021] | 0.397 0.482 0.577 | - - 0.457 | 0.246 0.383 | 0.540 - 0.344 | - - |
| QuatDE [Gao et al., 2021] | 0.438 0.509 0.586 | 1977 0.489 | 0.268 0.400 | 0.406 0.563 90 0.365 | - - |
| LineaRE [Peng and Zhang, 2020] | 0.453 0.509 0.578 | 1644 0.495 | 0.264 0.391 | 0.545 155 0.357 | - - |
| CapsE [Yu et al., 2019] | - - 0.559 | 718 0.415 | - - 0.356 403 0.150 | - - |
| RESCAL-DURA [Zhang et al., 2020b] | 0.455 - - 0.498 | 0.276 - - 0.550 - 0.368 | - - |
| HAKE [Zhang et al., 2020c] | 0.452 0.516 0.582 | - - 0.497 | 0.25 0.381 | - - 0.346 | - - |

### Table 2: Datasets statistics.

|        | WN18RR | FB15k-237 | UMLS |
|--------|--------|-----------|------|
| Entities | 40943  | 14541     | 135  |
| Relations | 11     | 237       | 46   |
| Train samples | 86835  | 272115    | 5216 |
| Valid samples | 3034   | 17535     | 652  |
| Test samples  | 3034   | 20466     | 661  |

We implement LP-BERT using Pytorch. Using a workstation with an Intel Xeon processor, 64GB of RAM and an Nvidia P40 GPU for training. We apply AdamW as an optimization algorithm with 5% steps of warmup. For the hyperparameters in LP-BERT, we set epochs=50, batch size=32, learning rate=10^{-4}/5 \times 10^{-5} respectively for the linear and attention parts initialized and set earlystop epoch num as 3. In knowledge graph fine-tuning phase, based on the best Hits@10 on dev set, we set batch size=64 on WN18RR, 120 on FB15k-237, 128 on UMLS, learning rate=10^{-4}/5 \times 10^{-5} respectively for the linear and attention parts initialized with LB-BERT, number of training epochs=7 on WN18RR and FB15k-237, 30 on UMLS, \(\alpha = 0.8\) on WN18RR and UMLS, \(\alpha = 0.5\) on FB15k-237, and \(\gamma = 2\) in Eq 11. We also set the
early stop epoch as 1.

As for valuation metrics, in the inference phase, given a test triple as the correct candidate, all other entities in the knowledge graph as the wrong candidate damage their head or tail entities. The trained model aims to use the ‘filtered’ settings to correct triple ranking of the corrupt. The evaluation metrics has two aspects: (1) Hits@N represents the ratio of test instances in the top N of correct candidates; (2) The average rank (MR) and the average reciprocal rank (MRR) reflect the absolute ranking.

4.2 Experimental Results

The link prediction results of competitive approaches and ours on the benchmark are shown in Table 1. It is observed our proposed LB-BERT is able to achieve state-of-the-art or competitive performance on WN18RR, FB15k-237 and UMLS dataset. The improvement is especially significant in terms of Hits@10 and Hits@3 due to the great generalization performance of multi-task pre-training textual encoding approach, which will be further analyzed in the section below. Furthermore, LP-BERT surpasses all other methods by a large margin in terms of Hits@3, Hits@10 on WN18RR and Hits@10 on UMLS. Although it only achieves inferior performance on FB15k-237 dataset and Hits@1 and MRR of WN18RR dataset compared to translational distance models, it still remarkably outperforms other semantic matching models such as KG-BERT and StAR from the same genre by introducing structured knowledge. In particular, LB-BERT outperforms StAR [Wang et al., 2021], which is the previous state-of-art model, on all three datasets with only one-third parameters numbers of it.

The experimental results show that the semantic matching models perform well in the topK recall evaluation methods, but the Hits@1 result is significantly worse than the translation distance models. This is because features of the semantic matching models are based on text, which lead to the vector representation of similar entities in the text are close and difficult to distinguish. Although the Hit@1 result of translation distance models is very high, it does not understand the text semantics. For an entity with similar text semantics, translation distance models cannot understand. For some new entities that are not seen in the training set, the prediction results of translation distance models are basically random, and the semantic matching models are reliable, which is also the reason why Hit@3 and Hit@10 LP-BERT can far exceed the translation distance models to achieve state-of-art performance.

Since our approach is an update from the BERT based textual models, says KG-BERT and StAR, we compared LB-BERT with KG-BERT and StAR on WN18RR in detail, including different initializations. As shown in Table 3, our proposed LB-BERT consistently achieves superior performance over most metrics. The evaluation effect of the LB-BERT model based on RoBERTa-base has exceeded the evaluation effect of KG-BERT and StAR based on RoBERTa-large. As for empirical efficiency, due to the small number of model parameters and the strategy of negative sampling based on batch in the training process, it is observed our model is faster than KG-BERT an StAR despite training or inference.

4.3 Ablation Study

To explore each module’s contribution, we conducted an extensive ablation study about LP-BERT. As shown in Table 4, we performed ablation experiments on WN18RR dataset. First of all, remove each optimization we proposed and get the benchmark evaluation effect shown in the first line. After adding batch-based triple-style negative sampling strategy combined with focal-loss, the appropriate negative sampling ratio greatly improves the model evaluation effect, as shown in the second line. The original pre-training weights (BERT or RoBERTa pretrained weights) are not familiar with the corpus information of the link prediction task. After adding the pre-training strategy based on MLM, the evaluation effect is further improved. However, the pre-training method based on MLM strategy does not fully excavate the relationship information of triplets, and the multi-task pre-training strategy combined with MLM, MEM and MRM makes the model evaluation result optimal.

5 Conclusion and Future Work

We present a multi-task pre-training knowledge graph BERT, named LP-BERT, for link prediction, which not only uses MLM to learn the knowledge of context corpus, but also introduces Mask Entity Model (MEM) and Mask Relation Model (MRM) tasks to learn the relationship information of triplets. According to this method, the structural relationship informations are introduced into pre-training model after transformed into unstructured corpus informations. Experimental results on dataset demonstrate both the efficiency and effectiveness of LP-BERT. In future work, we will add more diverse pre-training tasks and increase the model parameter size to enable LP-BERT to store more graph knowledge.

Table 3: Comparisons with KG-BERT and StAR on WN18RR. “T/Ep” and “Infer” stand for time per training epoch and inference time on test set, separately. The time was collected on Tesla P40 without mixed precision.

Table 4: Ablation results of LP-BERT on WN18RR dataset.
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