Subsampling for Knowledge Graph Embedding Explained

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Abstract

In this article, we explain the recent advance of subsampling methods in knowledge graph embedding (KGE) starting from the original one used in word2vec.

1 Negative Sampling Loss

Knowledge graph completion (KGC) is a research topic for automatically inferring new links in a KG that are likely but not yet known to be true.

We denote a triplet representing entities $e_i$, $e_j$ and their relation $r_k$ as $(e_i, r_k, e_j)$. In a typical KGC task, the model receives a query $(e_i, r_k, ?)$ or $(?, r_k, e_j)$ and predicts the entity corresponding to $\color{red}?\color{black}$.

Knowledge graph embedding (KGE) is a well-known scalable approach for KGC. In KGE, a KGE model scores a triplet $(e_i, r_k, e_j)$ by using a scoring function $s_\theta(x, y)$. Due to the computational cost, training of $s_\theta(x, y)$ commonly relies on the following negative sampling loss function [Sun et al., 2019, Ahrabian et al., 2020]:

$$
\ell_{\text{base}} = -\frac{1}{|D|} \sum_{(x, y) \in D} \left[ \log(\sigma(s_\theta(x, y) + \gamma)) + \frac{1}{\nu} \sum_{y_i \sim p_n(y_i | x)} \log(\sigma(-s_\theta(x, y_i) - \gamma)) \right],
$$

(1)

where $D = \{(x_1, y_1), \cdots, (x_n, y_n)\}$ represents observables that follow $p_d(x, y)$, $p_n(y|x)$ is the noise distribution, $\sigma$ is the sigmoid function, $\nu$ is the number of negative samples per positive sample $(x, y)$, and $\gamma$ is a margin term.

2 Subsampling in Negative Sampling Loss

Eq. (1) is on the assumption that the NS loss function fits the model to the distribution $p_d(y|x)$ defined from the observed data. However, what the NS loss actually does is to fit the model to the true distribution $p'_d(y|x)$ that exists behind the observed data. To fill in the gap between $p_d(y|x)$ and $p'_d(y|x)$, Kamigaito and Hayashi [2022a,b] theoretically add $A(x, y)$ and $B(x)$ to Eq. (1) as follows:

$$
\ell_{\text{sub}} = -\frac{1}{|D|} \sum_{(x, y) \in D} \left[ A(x, y) \log(\sigma(s_\theta(x, y) + \gamma)) + \frac{1}{\nu} \sum_{y_i \sim p_n(y_i | x)} B(x) \log(\sigma(-s_\theta(x, y_i) - \gamma)) \right].
$$

(2)

In this formulation, we can consider several assumptions for deciding $A(x, y)$ and $B(x)$. We introduce the assumptions in the following subsections.

2.1 Subsampling in word2vec (Base)

As a basic subsampling approach, Sun et al. [2019] used the original word2vec-based method for KGE learning defined as follows:

$$
A(x, y) = B(x, y) = \frac{1}{\sqrt{|\#(x, y)|}} \frac{|D|}{\sum_{(x', y') \in D} \sqrt{|\#(x', y')|}},
$$

(3)

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1 We include the detailed derivation of this function in Appendix A.
Table 1: Evaluation results of Kamigaito and Hayashi [2022b] for each subsampling method on the FB15k-237, WN18RR, and YAGO3-10 datasets. \textit{Sub.} denotes subsampling, \textit{None} denotes model that did not use subsampling, \textit{Base} denotes Eq. (3), \textit{Freq} denotes Eq. (5), and \textit{Uniq} denotes Eq. (6).

| Model | Sub. | FB15k-237 | | | | WN18RR | | | | | | YAGO3-10 | | |
|-------|------|-----------|---|---|---|------|---|---|---|---|---|---|
|       |      | MRR | Hits@ | | | MRR | Hits@ | | | | MRR | Hits@ | | |
|       |      | 1 | 3 | 10 | | | 1 | 3 | 10 | | | 1 | 3 | 10 | |
| RESCAL | None | 17.2 | 9.9 | 18.1 | 31.8 | | 41.5 | 39.0 | 42.3 | 45.9 | | - | - | - | - |
|        | Base | 22.3 | 13.9 | 24.2 | 39.8 | | 43.3 | 40.7 | 44.5 | 48.2 | | - | - | - | - |
|        | Freq | 26.6 | 17.4 | 29.4 | 45.1 | | 44.1 | 41.1 | 45.6 | 49.5 | | - | - | - | - |
|        | Uniq | 26.6 | 17.6 | 29.3 | 44.9 | | 44.1 | 41.4 | 45.5 | 49.5 | | - | - | - | - |
| ComplEx | None | 22.4 | 14.0 | 24.2 | 39.5 | | 45.0 | 40.9 | 46.6 | 53.4 | | - | - | - | - |
|        | Base | 32.2 | 23.0 | 35.1 | 51.0 | | 47.1 | 42.8 | 48.9 | 55.7 | | - | - | - | - |
|        | Freq | 32.8 | 23.6 | 36.1 | 51.2 | | 47.6 | 43.3 | 49.3 | 56.3 | | - | - | - | - |
|        | Uniq | 32.7 | 23.5 | 35.8 | 51.3 | | 47.6 | 43.2 | 49.5 | 56.3 | | - | - | - | - |
| DistMult | None | 22.2 | 14.0 | 24.0 | 39.4 | | 42.4 | 38.3 | 43.6 | 51.0 | | - | - | - | - |
|        | Base | 30.8 | 22.1 | 33.6 | 48.4 | | 43.9 | 39.4 | 45.2 | 53.3 | | 51.2 | 41.5 | 57.6 | 68.3 |
|        | Freq | 29.9 | 21.2 | 32.7 | 47.5 | | 44.6 | 40.0 | 45.9 | 54.4 | | - | - | - | - |
|        | Uniq | 29.1 | 20.3 | 31.8 | 46.6 | | 44.6 | 39.9 | 46.2 | 54.3 | | - | - | - | - |
| TransE | None | 33.0 | 22.8 | 37.2 | 53.0 | | 22.6 | 1.8 | 40.1 | 52.3 | | 56.6 | 40.9 | 56.6 | 67.7 |
|        | Base | 32.9 | 23.0 | 36.8 | 52.7 | | 22.4 | 2.4 | 40.1 | 53.0 | | 52.1 | 41.5 | 57.6 | 68.3 |
|        | Freq | 33.6 | 24.0 | 37.3 | 52.9 | | 23.0 | 1.9 | 40.7 | 53.7 | | 51.3 | 41.9 | 57.2 | 68.1 |
|        | Uniq | 33.5 | 23.9 | 37.3 | 52.8 | | 23.2 | 2.2 | 41.0 | 53.4 | | 51.4 | 42.0 | 57.6 | 67.9 |
| RotatE | None | 33.1 | 23.1 | 37.1 | 53.1 | | 47.3 | 42.6 | 49.1 | 56.7 | | 50.6 | 41.1 | 56.5 | 67.8 |
|        | Base | 33.6 | 23.9 | 37.4 | 53.2 | | 47.6 | 43.1 | 49.5 | 56.6 | | 50.8 | 41.8 | 56.5 | 67.6 |
|        | Freq | 34.0 | 24.5 | 37.6 | 53.2 | | 47.8 | 42.9 | 49.8 | 57.4 | | 51.0 | 41.9 | 56.5 | 67.8 |
|        | Uniq | 34.0 | 24.5 | 37.6 | 53.0 | | 47.9 | 43.5 | 49.6 | 56.7 | | 51.5 | 42.5 | 56.8 | 68.3 |
| HAKE | None | 32.3 | 21.6 | 36.9 | 53.2 | | 49.1 | 44.5 | 51.1 | 57.8 | | 53.4 | 44.9 | 58.7 | 68.4 |
|        | Base | 34.5 | 24.7 | 38.2 | 54.3 | | 49.8 | 45.3 | 51.6 | 58.2 | | 54.3 | 46.1 | 59.5 | 69.2 |
|        | Freq | 34.9 | 25.2 | 38.6 | 54.2 | | 49.7 | 45.2 | 51.4 | 58.5 | | 54.0 | 45.5 | 59.4 | 69.1 |
|        | Uniq | 35.4 | 25.8 | 38.9 | 54.7 | | 49.8 | 45.4 | 51.5 | 58.3 | | 55.0 | 46.6 | 60.1 | 69.8 |

where \# is the symbol for frequency and \#(x, y) represents the frequency of (x, y)^2. Note that the actual (x, y) occurs at most once in the KG, so when (x, y) = (e_i, r_k, e_j), they approximate the frequency of (x, y) as follows:

\[
\#(x, y) \approx \#(e_i, r_k) + \#(r_k, e_j).
\]

Different from the form in Eq. (2), Eq. (3) use A(x, y) and B(x, y), instead of A(x, y) and B(x). Thus, their approach does not follow the theoretically induced loss function in Eq. (2).

### 2.2 Frequency-based Subsampling (Freq)

Frequency-based subsampling [Kamigaito and Hayashi, 2022b] is based on the assumption that in \( p_{\theta}(y|x) \), (x, y) originally has a frequency, but the observed one is at most 1. Since A(x, y) needs to discount the frequency of (x, y), and B(x) needs to discount that of x, we can derive the following subsampling method based on word2vec [Mikolov et al., 2013] as implemented by the previous work [Sun et al., 2019]^3:

\[
A(x, y) = \frac{1}{\sqrt{\#(x, y)}} |D|, \quad B(x) = \frac{1}{\sqrt{\#x}} |D| \sum_{x' \in D} \frac{1}{\sqrt{\#(x', y')}}.
\]

^2In the original word2vec, they randomly discard a word by a probability \( 1 - \frac{1}{\sqrt{f}} \), where t is a constant value and f is a frequency of a word. This is similar to randomly keep a word with a probability \( \sqrt{f} \).

^3https://github.com/DeepGraphLearning/KnowledgeGraphEmbedding
2.3 Unique-based Subsampling (Uniq)

In the true distribution $p'_d(y|x)$, however, if we assume that $(x, y)$ has frequency 1 at most, as in the observation, then $p'_d(y|x) = p'_d(x, y)/p'_d(x) \propto 1/p'_d(x)$, so $p'_d(y|x)$ is the same for an $x$ independent from $y$. Therefore, under this assumption, we have only need to consider a discount for $p'_d(x)$ and can derive the unique-based subsampling [Kamigaito and Hayashi, 2022b] as follows:

$$A(x, y) = B(x) = \frac{1}{\sqrt{\sum_{x' \in D} 1/\sqrt{p'_d(x')}}}.$$  

(6)

3 Effectiveness of Subsampling in KGE

We conducted experiments to evaluate our subsampling methods. We used FB15k-237 [Toutanova and Chen, 2015], WN18RR, and YAGO3-10 [Dettmers et al., 2018] for the evaluation. As comparison methods, we used ComplEx [Trouillon et al., 2016], RESCAL [Bordes et al., 2011], DistMult [Yang et al., 2015], TransE [Bordes et al., 2013], RotatE [Sun et al., 2019], and HAKE [Zhang et al., 2020]. We followed the original settings of Sun et al. [2019] for ComplEx, DistMult, TransE, and RotatE with their implementation\(^4\)\(^5\) and the original settings of Zhang et al. [2020] for HAKE with their implementation\(^5\). In RESCAL, we inherited the original setting of DistMult and set the dimension size to 500 for saving computational time. Since Kamigaito and Hayashi [2021] refer to the smoothing effect of self-adversarial negative sampling (SANS) [Sun et al., 2019] that is a role of subsampling, we applied subsampling on SANS for investigating the performance in practical settings.

Table 1 shows the result. We can see that subsampling improved KG completion performances from the methods without subsampling. Furthermore, frequency-based and unique-based subsampling basically outperformed the baseline subsampling.

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Hidetaka Kamigaito and Katsuhiko Hayashi. Unified interpretation of softmax cross-entropy and negative sampling: With case study for knowledge graph embedding. In Proceedings of the 59th Annual Meeting of the Association for Computational Linguistics and the 11th International Joint Conference on Natural Language Processing (Volume 1: Long Papers), pages 5517–5531, Online, August 2021. Association for Computational Linguistics. doi: 10.18653/v1/2021.acl-long.429. URL https://aclanthology.org/2021.acl-long.429.

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\(^4\)https://github.com/DeepGraphLearning/KnowledgeGraphEmbedding

\(^5\)https://github.com/MIRALab-USTC/KGE-HAKE
Hidetaka Kamigaito and Katsuhiko Hayashi. Comprehensive analysis of negative sampling in knowledge graph representation learning. In Proceedings of the 39th International Conference on Machine Learning, volume 162 of Proceedings of Machine Learning Research, pages 10661–10675. PMLR, 17–23 Jul 2022b. URL https://arxiv.org/abs/2206.10140.

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A  The Detailed Derivation of Eq. (2)

We can reformulate the NS loss in Eq. (1) as follows:

\[
(1) = - \frac{1}{|D|} \sum_{(x,y) \in D} \left[ \log(\sigma(s_\theta(x,y) + \gamma)) + \frac{1}{\nu} \sum_{y_i \sim p_n(y|x)} \log(\sigma(-s_\theta(x,y_i) - \gamma)) \right]
\]

\[
= - \frac{1}{|D|} \sum_{(x,y) \in D} \log(\sigma(s_\theta(x,y) + \gamma)) - \frac{1}{|D|} \sum_{(x,y) \in D} \frac{1}{\nu} \sum_{y_i \sim p_n(y|x)} \log(\sigma(-s_\theta(x,y_i) - \gamma)). \tag{7}
\]

Here, we can consider the following approximation based on the Monte Carlo method:

\[
\frac{1}{\nu} \sum_{y_i \sim p_n(y|x)} \log(\sigma(-s_\theta(x,y_i) - \gamma)) \approx \sum_y p_n(y|x) \log(\sigma(-s_\theta(x,y) - \gamma)). \tag{8}
\]

Using Eq. (8), we can reformulate Eq. (7) as follows:

\[
(7) \approx - \frac{1}{|D|} \sum_{(x,y) \in D} \log(\sigma(s_\theta(x,y) + \gamma)) - \frac{1}{|D|} \sum_{(x,y) \in D} \sum_{y'} p_n(y'|x) \log(\sigma(-s_\theta(x,y') - \gamma)). \tag{9}
\]

Similar to Eq. (8), we can consider the following approximation by the the Monte Carlo method:

\[
- \frac{1}{|D|} \sum_{(x,y) \in D} \log(\sigma(s_\theta(x,y) + \gamma)) \approx - \sum_{x,y} \log(\sigma(s_\theta(x,y) + \gamma)) p_d(x,y),
\]

\[
- \frac{1}{|D|} \sum_{(x,y) \in D} \sum_{y'} p_n(y'|x) \log(\sigma(-s_\theta(x,y') - \gamma)) \approx - \sum_x \sum_{y'} p_n(y'|x) \log(\sigma(-s_\theta(x,y') - \gamma)) p_d(x). \tag{10}
\]

Using Eq. (10), we can reformulate Eq. (9) as follows:

\[
(9) \approx - \sum_{x,y} \log(\sigma(s_\theta(x,y) + \gamma)) p_d(x,y) - \sum_{x,y} \sum_{y'} p_n(y'|x) \log(\sigma(-s_\theta(x,y') - \gamma)) p_d(x)
\]

\[
= - \sum_{x,y} \log(\sigma(s_\theta(x,y) + \gamma)) p_d(x,y) - \sum_{x,y} p_n(y|x) \log(\sigma(-s_\theta(x,y) - \gamma)) p_d(x)
\]

\[
= - \sum_{x,y} \left[ \log(\sigma(s_\theta(x,y) + \gamma)) p_d(x,y) + p_n(y|x) \log(\sigma(-s_\theta(x,y) - \gamma)) p_d(x) \right]. \tag{11}
\]

Next, we consider replacements of \(p_d(x,y)\) with \(p_d'(x,y)\) and \(p_d(x)\) with \(p_d'(x)\). By assuming two functions, \(A(x,y)\) and \(B(x)\), that convert \(p_d(x,y)\) into \(p_d'(x,y)\) and \(p_d(x)\) into \(p_d'(x)\), we further reformulate Eq. (11) as follows:

\[
- \sum_{x,y} \left[ \log(\sigma(s_\theta(x,y) + \gamma)) p_d'(x,y) + p_n(y|x) \log(\sigma(-s_\theta(x,y) - \gamma)) p_d'(x) \right]
\]

\[
= - \sum_{x,y} \left[ \log(\sigma(s_\theta(x,y) + \gamma)) A(x,y) p_d'(x,y) + p_n(y|x) \log(\sigma(-s_\theta(x,y) - \gamma)) B(x) p_d'(x) \right]. \tag{12}
\]

Based on the similar derivation from Eq. (1) to Eq. (11), we can reformulate Eq. (12) as follows:

\[
(12) \approx - \frac{1}{|D|} \sum_{(x,y) \in D} \left[ A(x,y) \log(\sigma(s_\theta(x,y) + \gamma)) + \frac{1}{\nu} \sum_{y_i \sim p_n(y|x)} B(x) \log(\sigma(-s_\theta(x,y_i) - \gamma)) \right]. \tag{13}
\]