Learning Representations of Bi-level Knowledge Graphs for Reasoning beyond Link Prediction*

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Abstract

Knowledge graphs represent known facts using triplets. While existing knowledge graph embedding methods only consider the connections between entities, we propose considering the relationships between triplets. For example, let us consider two triplets T_1 and T_2 where T_1 is (Academy_Awards, Nominates, Avatar) and T_2 is (Avatar, Wins, Academy_Awards). Given these two base-level triplets, we see that T_1 is a prerequisite for T_2 . In this paper, we define a higher-level triplet to represent a relationship between triplets, e.g., $\langle T_1, \text{ PrerequisiteFor, } T_2 \rangle$ where Prerequisite-For is a higher-level relation. We define a bi-level knowledge graph that consists of the base-level and the higher-level triplets. We also propose a data augmentation strategy based on the random walks on the bi-level knowledge graph to augment plausible triplets. Our model called BiVE learns embeddings by taking into account the structures of the base-level and the higher-level triplets, with additional consideration of the augmented triplets. We propose two new tasks: triplet prediction and conditional link prediction. Given a triplet T_1 and a higher-level relation, the triplet prediction predicts a triplet that is likely to be connected to T_1 by the higher-level relation, e.g., $\langle T_1, \text{PrerequisiteFor}, ? \rangle$. The conditional link prediction predicts a missing entity in a triplet conditioned on another triplet, e.g., $\langle T_1, PrerequisiteFor, (Avatar, Wins, ?) \rangle$. Experimental results show that BiVE significantly outperforms all other methods in the two new tasks and the typical baselevel link prediction in real-world bi-level knowledge graphs.

Introduction

A knowledge graph represents the relationships between entities using triplets consisting of a head entity, a relation, and a tail entity. Knowledge graph embedding aims to represent the entities and relations as a set of embedding vectors that can be utilized in many modern AI applications [16, 19]. Most existing knowledge graph embedding methods generate the embedding vectors by focusing solely on how the entities are connected by the relations [4, 5, 34]. Even though some methods predict missing connections between the entities by rule mining [25, 29] or rule-and-path-based learning [27], these exist-

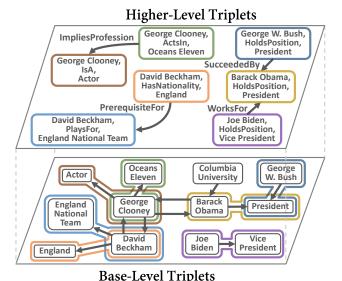


Figure 1: Example of a bi-level knowledge graph consisting of base-level and higher-level triplets in the *FBHE* dataset. The relation labels are omitted in the base-level triplets.

ing approaches only enable expanding the entity-level connections.

Each triplet in a knowledge graph can have a relationship with another triplet. For example, let us consider two baselevel triplets T_1 and T_2 where T_1 is (Joe_Biden, HoldsPosition, Vice_President) and T2 is (Barack_Obama, HoldsPosition, President). To represent the fact that Joe Biden was a vice president when Barack Obama was a president, we define a higher-level triplet $\langle T_1, \text{WorksFor}, T_2 \rangle$ where WorksFor is a higher-level relation. In this paper, we define a bi-level knowledge graph that includes both the base-level and the higherlevel triplets, where the base-level triplets correspond to the original triplets representing the relationships between entities, while the higher-level triplets represent the relationships between the base-level triplets using the higher-level relations. Based on well-known knowledge graphs, FB15K237 [32] and DB15K [10], we create three real-world bi-level knowledge graphs named FBH, FBHE, and DBHE. Figure 1 shows a subgraph of a bi-level knowledge graph in FBHE where the baselevel triplets correspond to the original triplets in FB15K237 and the higher-level triplets are manually created by defining

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the higher-level relationships between the base-level triplets.

We propose incorporating the base-level and the higherlevel triplets into knowledge graph embedding. Using the bilevel knowledge graphs, we also propose a data augmentation strategy that augments triplets by identifying plausible relation sequences based on random walks. We develop a new knowledge graph embedding method called BiVE (embedding of Bile**V**el knowledg**E** graphs) that computes embedding vectors by reflecting the structures of the base-level and the higherlevel triplets simultaneously, where the augmented triplets are further incorporated. Using the bi-level knowledge graphs, we propose two new tasks: triplet prediction and conditional link prediction. The triplet prediction predicts a triplet that is likely to be connected to a given triplet using a higher-level relation, e.g., $\langle T_1, \text{WorksFor}, ? \rangle$, whereas the conditional link prediction predicts a missing entity in a triplet where another triplet is provided as a condition, e.g., $\langle T_1, WorksFor, (?, HoldsPo$ sition, President). Experimental results show that BiVE significantly outperforms other state-of-the-art knowledge graph completion methods in real-world datasets.¹

Our contributions can be summarized as follows:

- To the best of our knowledge, our work is the first work that introduces the higher-level relationships between triplets in knowledge graphs; we define bi-level knowledge graphs and create three real-world datasets.
- We propose an efficient data augmentation strategy using random walks on a bi-level knowledge graph.
- We develop BiVE to learn embeddings by effectively incorporating the base-level triplets, the higher-level triplets, and the augmented triplets.
- We propose two new tasks, triplet prediction and conditional link prediction, which have never been studied.
- BiVE significantly outperforms 12 different state-of-theart knowledge graph completion methods.

Related Work

Some knowledge graph completion methods use multi-hop paths between distant entities [6, 17, 22, 23, 27] and rulebased or logic-based methods identify frequently observed patterns [7, 12, 25, 26, 29, 37]. The main difference between these methods and BiVE is that the existing methods only consider the relationships between entities, whereas BiVE considers not only the relationships between entities but also the relationships between triplets. Also, the way of expressing the relationships between entities or triplets in BiVE is not restricted to the first-order-logic-like expression. For example, the rulebased methods consider the relationships between connected entities, e.g., $\forall x, y, z : (x, r_1, y) \land (y, r_2, z) \Rightarrow (x, r_3, z)$ where there should exist a path connecting x, y, and z in the knowledge graph. On the other hand, BiVE represents relationships like $(x, r_1, y) \stackrel{\widehat{r}}{\Rightarrow} (p, r_2, q)$ where x, y and p, q are not necessarily connected by the base-level triplets, and also r_1 , r_2 , and $\stackrel{\widehat{r}}{\Rightarrow}$ can be any relation not restricted to the first-order-logic-like relation.

Even though there have been many attempts to discover meaningful patterns in a knowledge graph and utilize them to complete missing links [20], such attempts have rarely been studied in the context of data augmentation. Recently, rule-based data augmentation for knowledge graph embedding has been proposed [21]². While this method uses logical rules using the base-level triplets, our data augmentation employs random walks on a bi-level knowledge graph.

To exploit enriched information about triplets, some knowledge graph embedding methods utilize attributes of entities or ontological concepts [14]. TransEA [35] considers numeric attributes of entities, and LiteralE [18] considers information from literals. HINGE [28] has been proposed to represent hyper-relational facts where a triplet has additional key-value pairs to present extra information about each triplet. Even though these methods consider enriched information about triplets, they do not consider the relationships between triplets.

In information retrieval, a neural fact contextualization method has been proposed to rank a set of candidate facts for a given triplet [33]. Also, a way of representing a triplet in an embedding space is studied by considering the concept of a line graph [9]. Recently, ATOMIC [30] has been proposed to provide commonsense knowledge for if-then reasoning, whereas ASER [39] has been proposed to construct an eventuality knowledge graph. Although these methods consider triplet-level operations, the goal of their methods is different from ours and none of these considers the bi-level knowledge graphs.

Bi-Level Knowledge Graphs

Let us represent a knowledge graph as $G=(\mathcal{V},\mathcal{R},\mathcal{E})$ where \mathcal{V} is a set of entities, \mathcal{R} is a set of relations, and $\mathcal{E}=\{(h,r,t):h\in\mathcal{V},r\in\mathcal{R},t\in\mathcal{V}\}$ is a set of triplets. Let us call G a base-level knowledge graph and call $(h,r,t)\in\mathcal{E}$ a base-level triplet. We formally define the higher-level triplets as follows.

Definition 1 (Higher-Level Triplets) Given a base-level knowledge graph $G = (\mathcal{V}, \mathcal{R}, \mathcal{E})$, a set of higher-level triplets is defined by $\mathcal{H} = \{\langle T_i, \widehat{r}, T_j \rangle : T_i \in \mathcal{E}, \widehat{r} \in \widehat{\mathcal{R}}, T_j \in \mathcal{E}\}$ where \mathcal{E} is a set of base-level triplets and $\widehat{\mathcal{R}}$ is a set of higher-level relations connecting the base-level triplets.

We define a bi-level knowledge graph as follows.

Definition 2 (Bi-Level Knowledge Graph) Given a base-level knowledge graph $G = (\mathcal{V}, \mathcal{R}, \mathcal{E})$, a set of higher-level relations $\widehat{\mathcal{R}}$, and a set of higher-level triplets \mathcal{H} , a bi-level knowledge graph is defined as $\widehat{G} = (\mathcal{V}, \mathcal{R}, \mathcal{E}, \widehat{\mathcal{R}}, \mathcal{H})$.

¹https://github.com/bdi-lab/BiVE

²We could not include this method as a baseline in our experiments because the authors of [21] could not provide their source codes due to some confidentiality restrictions.

\widehat{r}		$\langle T_i, \widehat{r}, T_j angle$
Prerequi	siteFor	$T_i \colon (\text{BAFTA_Award, Nominates, The_King's_Speech})$ $T_j \colon (\text{The_King's_Speech, Wins, BAFTA_Award})$
ImpliesPr	ofession	T _i : (Liam_Neeson, ActsIn, Love_Actually) T _i : (Liam_Neeson, IsA, Actor)
Works	sFor	T _i : (Joe_Biden, HoldsPosition, Vice_President) T _i : (Barack_Obama, HoldsPosition, President)
Succeed	edBy	T _i : (George_W.Bush, HoldsPosition, President) T _i : (Barack_Obama, HoldsPosition, President)
ImpliesTi	meZone	T_i^* : (Czech_Republic, TimeZone, Central_European) T_i : (Prague, TimeZone, Central_European)
NextAlm	aMater	T_i : (Gerald Ford, StudiesIn, University of Michigan) T_j : (Gerald Ford, StudiesIn, Yale University)

Table 1: Examples of Higher-Level Relations and Triplets.

To define a bi-level knowledge graph, we add the higherlevel triplets \mathcal{H} to the base-level knowledge graph G by introducing the higher-level relations R. We create real-world bilevel knowledge graphs FBH and FBHE based on FB15K237 from Freebase [2] and DBHE based on DB15K from DBpedia [1]. Table 1 shows some examples of the higher-level relations and triplets. FBH contains the higher-level relations that can be inferred inside the base-level knowledge graph, e.g., PrerequisiteFor and ImpliesProfession, whereas FBHE and DBHE contain some externally-sourced knowledge, e.g., WorksFor and NextAlmaMater. For example, we crawl Wikipedia articles to find information about the (vice)presidents of the United States and the alma mater information of politicians. As a result, FBH contains six different higher-level relations, FBHE has ten higher-level relations, and DBHE has eight higher-level relations. Note that the base-level knowledge graphs of FBH and FBHE are FB15K237. FBHE extends FBH by including the externallysourced higher-level relationships. The authors of this paper manually defined the higher-level relations and added the higher-level triplets to FB15K237 and DB15K, which took six weeks.

Using a bi-level knowledge graph, we define the triplet prediction problem as follows.

Definition 3 (Triplet Prediction) Given a bi-level knowledge graph $\widehat{G} = (\mathcal{V}, \mathcal{R}, \mathcal{E}, \widehat{\mathcal{R}}, \mathcal{H})$ where $\mathcal{H} = \{\langle T_i, \widehat{r}, T_j \rangle : T_i \in \mathcal{E}, \widehat{r} \in \widehat{\mathcal{R}}, T_j \in \mathcal{E}\}$, the triplet prediction problem is defined as $\langle T_i, \widehat{r}, \widehat{r}, \rangle$ or $\langle \widehat{r}, \widehat{r}, T_j \rangle$ where the goal is to predict the missing base-level triplet.

Also, we define the conditional link prediction as follows.

Definition 4 (Conditional Link Prediction) Given a bi-level knowledge graph $\widehat{G} = (\mathcal{V}, \mathcal{R}, \mathcal{E}, \widehat{\mathcal{R}}, \mathcal{H})$ where $\mathcal{H} = \{\langle T_i, \widehat{r}, T_j \rangle : T_i \in \mathcal{E}, \widehat{r} \in \widehat{\mathcal{R}}, T_j \in \mathcal{E} \}$, let $T_i \coloneqq (h_i, r_i, t_i)$ and $T_j \coloneqq (h_j, r_j, t_j)$. The conditional link prediction problem is to predict a missing entity in a base-level triplet conditioned on another base-level triplet. Specifically, the problem is defined as $\langle T_i, \widehat{r}, (h_j, r_j, ?) \rangle$ or $\langle T_i, \widehat{r}, (r_j, r_j, t_j) \rangle$ or $\langle T_i, r_j, r_j, r_j \rangle$ or $\langle T_i, r_j, r_j, r_j \rangle$.

Data Augmentation by Random Walks on a Bi-Level Knowledge Graph

Consider a bi-level knowledge graph in the training set $\widehat{G}_{\text{train}} = (\mathcal{V}, \mathcal{R}, \mathcal{E}_{\text{train}}, \widehat{\mathcal{R}}, \mathcal{H}_{\text{train}})$ where $\mathcal{E}_{\text{train}}$ and $\mathcal{H}_{\text{train}}$ are the base-level and the higher-level triplets in the training set respectively. We add reverse relations to \mathcal{R} and add reversed triplets to $\mathcal{E}_{\text{train}}$, i.e., for every $r \in \mathcal{R}$, we add r^{-1} that has the reverse direction of r and for every $(h,r,t) \in \mathcal{E}_{\text{train}}$, we add (t,r^{-1},h) to $\mathcal{E}_{\text{train}}$. Similarly, for every $\widehat{r} \in \widehat{\mathcal{R}}$, we add \widehat{r}^{-1} and add the reversed higher-level triplets to $\mathcal{H}_{\text{train}}$. All these reverse relations and reversed triplets are added only for data augmentation.

From an entity h, we randomly visit one of its neighbors by following a base-level or a higher-level triplet. To search for diverse patterns, we do not allow going back to an entity that has already been visited. Let us define a random walk path to be the sequence of visited entities, visited relations, and visited higher-level relations. Consider two baselevel triplets $T_i = (h_i, r_i, t_i)$ and $T_j = (h_j, r_j, t_j)$ and a higher-level triplet $\langle T_i, \hat{r}, T_j \rangle$. From any entity in T_i , we can go to any entity in T_i and vice versa by following r_i , \hat{r} , and r_j or their reverse relations. For example, one possible random walk path is $(h_i, r_i, \hat{r}, r_j, t_j)$. Another possible random walk path is $(t_j, r_j^{-1}, \hat{r}^{-1}, r_i, t_i)$. Assume that we have a base-level triplet $T_0 = (h_0, r_0, h_i)$. Starting from h_0 , we can make a longer path, e.g., $(h_0, r_0, h_i, r_i, \hat{r}, r_i, t_i)$. We define the length of a random walk path to be the number of entities in the sequence except the starting entity.

Given the maximum length of a random walk path L, we repeat the random walks by varying the length $l=2,\cdots,L$ and repeat the random walks n times for every l. In our experiments, we set L=3 and n=50,000,000. Let w denote the sequence of a random walk path of all possible lengths, where we randomly select a starting entity for every w. If there are multiple identical random walk paths, we remove the duplicates to prevent unexpected bias. Let p_k be the k-th unique sequence of relations and higher-level relations extracted from w, i.e., we make p_k by removing all entities from w, e.g., if $w=(h_0,r_0,h_i,r_i,\widehat{r},r_j,t_j)$ then $p_k=(r_0,r_i,\widehat{r},r_j)$. We call p_k the relation sequence. Since p_k only traces the relations, different random walk paths can be mapped into the same p_k . Using p_k , we rewrite a random walk path $w=(h,\cdots,t)$ to $w = (h, p_k, t)$ where the relation sequence of the original path w is mapped into p_k , h is the starting entity and t is the last entity. Let W denote the multiset of all random walk paths of all possible lengths. We define the confidence score of (p_k, r)

$$c(p_k,r) \coloneqq \frac{|\{(h,r,t): (h,p_k,t) \in \mathcal{W}, (h,r,t) \in \mathcal{E}_{\text{train}}\}|}{|\{(h,p_k,t): (h,p_k,t) \in \mathcal{W}\}|}.$$

We select the pairs of (p_k, r) that satisfies $c(p_k, r) \ge \tau$ where we set $\tau = 0.7$. Let $\mathcal{S}_{kr} := \{(h, r, t) : (h, p_k, t) \in \mathcal{W}, c(p_k, r) \ge \tau, (h, r, t) \notin \mathcal{E}_{\text{train}}\}$ where \mathcal{S}_{kr} indicates a set of missing triplets (h, r, t) even though $c(p_k, r) \ge \tau$. Then, let

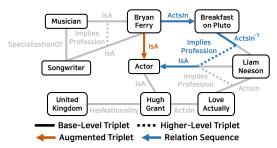


Figure 2: Random walk path in a bi-level knowledge graph and an augmented triplet in *FBH*. We add missing triplets whose confidence scores are greater than a certain threshold.

 $\mathcal{S} := \cup_k \cup_r \mathcal{S}_{kr}$ where \mathcal{S} is a set of augmented triplets. We add the triplets in \mathcal{S} to a bi-level knowledge graph to augment triplets that are likely to be present. Figure 2 shows an example of a random walk path of length 2 and an augmented triplet in FBH, where the walk starts from Bryan_Ferry. Let $p_1 = (ActsIn, ActsIn^{-1}, ImpliesProfession, IsA)$. Since the confidence score of (p_1, IsA) is 0.99, we add a triplet (Bryan_Ferry, IsA, Actor) which was missing in the original training set.

Embedding of Bi-Level Knowledge Graphs

A knowledge graph embedding method defines a scoring function $f(\mathbf{h}, \mathbf{r}, \mathbf{t})$ of a triplet (h, r, t), where \mathbf{h}, \mathbf{r} , and \mathbf{t} are embedding vectors of h, r, and t respectively; a higher score indicates a more plausible triplet. In BiVE, the loss incurred by the base-level triplets, L_{base} , is defined as follows:

$$L_{\text{base}} \coloneqq \sum_{(h,r,t) \in \mathcal{E}_{\text{train}}} g(-f(\mathbf{h},\mathbf{r},\mathbf{t})) + \sum_{(h',r',t') \in \mathcal{E}'_{\text{train}}} g(f(\mathbf{h}',\mathbf{r}',\mathbf{t}'))$$

where $g(x) = \log(1 + \exp(x))$ and $\mathcal{E}'_{\text{train}}$ is a set of corrupted triplets. We can use any knowledge graph embedding scoring function for $f(\cdot)$. We implement BiVE with two different scoring functions for $f(\cdot)$: QuatE [40] for BiVE-Q and BiQUE [11] for BiVE-B.

Given $T_i = (h_i, r_i, t_i)$, let \mathbf{T}_i denote an embedding vector of T_i where the dimension is \hat{d} . We define $\mathbf{T}_i \coloneqq \mathbf{W}[\mathbf{h}_i; \mathbf{r}_i; \mathbf{t}_i]$ where \mathbf{h}_i , \mathbf{r}_i , and \mathbf{t}_i denote the embedding vectors of h_i , r_i , and t_i respectively, the dimension of each of these embedding vectors is d, and \mathbf{W} is a projection matrix of size $\hat{d} \times 3d$ which projects the vertically concatenated vector to the \hat{d} -dimensional space. Similarly, $\mathbf{T}_j = \mathbf{W}[\mathbf{h}_j; \mathbf{r}_j; \mathbf{t}_j]$ where $T_j = (h_j, r_j, t_j)$. We define the loss incurred by the higher-level triplets, L_{high} , as follows:

$$L_{\mathrm{high}} \coloneqq \sum_{\langle T_i, \widehat{r}, T_j \rangle} g(-f(\mathbf{T}_i, \widehat{\mathbf{r}}, \mathbf{T}_j)) + \sum_{\langle {T_i}', \widehat{r}', {T_j}' \rangle} g(f(\mathbf{T}_i', \widehat{\mathbf{r}}', \mathbf{T}_j'))$$

where $\langle T_i, \widehat{r}, T_j \rangle \in \mathcal{H}_{\text{train}}$, $\langle T_i', \widehat{r}', T_j' \rangle \in \mathcal{H}'_{\text{train}}$, $\widehat{\mathbf{r}}$ is the embedding vector of \widehat{r} , the dimension of $\widehat{\mathbf{r}}$ is \widehat{d} , and $\langle T_i', \widehat{r}', T_j' \rangle$ is a corrupted higher-level triplet made by randomly replacing T_i or T_j with one of the triplets in $\mathcal{E}_{\text{train}}$.

We define the loss of the augmented triplets, L_{aug} , as

	$ \mathcal{V} $	$ \mathcal{R} $	$ \mathcal{E} $	$ \widehat{\mathcal{R}} $	$ \mathcal{H} $	$ \widehat{\mathcal{E}} $
FBH	14,541	237	310,117	6	27,062	33,157
<i>FBHE</i>	14,541	237	310,117	10	34,941	33,719
DBHE	12,440	87	68,296	8	6,717	8,206

Table 2: Statistics of a bi-level knowledge graph $\widehat{G}=(\mathcal{V},\mathcal{R},\mathcal{E},\widehat{\mathcal{R}},\mathcal{H}).\,|\widehat{\mathcal{E}}|$ is the number of base-level triplets which are involved in the higher-level triplets.

$$L_{\text{aug}} := \sum_{(h,r,t) \in \mathcal{S}} g(-f(\mathbf{h},\mathbf{r},\mathbf{t})) + \sum_{(h',r',t') \in \mathcal{S}'} g(f(\mathbf{h'},\mathbf{r'},\mathbf{t'}))$$

where S is the set of the augmented triplets and S' is the set of corrupted triplets.

Finally, our loss function of BiVE is defined by

$$L_{\text{BiVE}} \coloneqq L_{\text{base}} + \lambda_1 \cdot L_{\text{high}} + \lambda_2 \cdot L_{\text{aug}}$$

where λ_1 is a hyperparameter indicating the importance of the higher-level triplets and λ_2 indicates the importance of the augmented triplets. By optimizing $L_{\rm BiVE}$, BiVE learns embeddings by considering the structures of the base-level triplets, the higher-level triplets, and the augmented triplets.

Let us describe the scoring functions of BiVE for triplet prediction and conditional link prediction. To solve a triplet prediction problem, $\langle T_i, \widehat{r}, ? \rangle$, we compute $F_{\rm tp}(X) := f(\mathbf{T}_i, \widehat{\mathbf{r}}, \mathbf{X})$ for every base-level triplet $X \in \mathcal{E}_{\rm train}$ where \mathbf{X} is a learned embedding vector of X. To solve a conditional link prediction problem, $\langle T_i, \widehat{r}, (h_j, r_j, ?) \rangle$, we compute $F_{\rm clp}(x) := f(\mathbf{h}_j, \mathbf{r}_j, \mathbf{x}) + \lambda_1 \cdot f(\mathbf{T}_i, \widehat{\mathbf{r}}, \boldsymbol{W}[\mathbf{h}_j; \mathbf{r}_j; \mathbf{x}])$ for every $x \in \mathcal{V}$ where \mathbf{x} is a learned embedding of x.

Experimental Results

We use three real-world bi-level knowledge graphs presented in Table 2, where $|\hat{\mathcal{E}}|$ is the number of base-level triplets involved in the higher-level triplets. We split \mathcal{E} and \mathcal{H} into training, validation, and test sets with a ratio of 8:1:1. We use three standard evaluation metrics: the filtered MR (Mean Rank), MRR (Mean Reciprocal Rank), and Hit@10 [34]. Higher MRR and Hit@10 and a lower MR indicate better results. We repeat experiments ten times for each method and report the mean and the standard deviation. We set d = 200 and d = 200200. We use 12 different baseline methods: ASER [39], MIN-ERVA [6], Multi-Hop [22], Neural-LP [37], DRUM [29], Any-BURL [25], PTransE [23], RPJE [27], TransD [15], ANAL-OGY [24], QuatE [40] and BiQUE [11]. For TransD and ANALOGY, we use the implementations in OpenKE [13]. More details of datasets and methods are described in the Supplementary Material.

Triplet Prediction

While BiVE solves a triplet prediction problem using the scoring function $F_{\rm tp}(X)$, none of the baseline methods can deal with the higher-level triplets. To feed the higher-level triplets to the baseline methods, we create a new knowledge graph G_T where a base-level triplet is converted into an entity and a higher-level triplet is converted into a triplet. Let

		FBH			FBHE			DBHE	
	MR (↓)	MRR (†)	Hit@10 (†)	MR (↓)	MRR (†)	Hit@10 (†)	MR (↓)	MRR (†)	Hit@10 (†)
ASER	74541.7 ± 0.0	0.011 ± 0.000	0.015±0.000	57916.0 ± 0.0	0.050 ± 0.000	0.070 ± 0.000	18157.6 ± 0.0	0.042 ± 0.000	0.075 ± 0.000
MINERVA	109055.1 ± 98.5	$0.093\!\pm\!0.002$	$0.113 {\pm} 0.002$	$85571.5 {\pm} 768.3$	0.220 ± 0.008	0.300 ± 0.005	20764.3 ± 72.3	0.177 ± 0.005	0.221 ± 0.004
Multi-Hop	108731.7 ± 43.2	$0.105 \!\pm\! 0.001$	$0.117 {\pm} 0.000$	83643.8 ± 33.2	$0.255 {\pm} 0.012$	$0.311 {\pm} 0.003$	20505.8 ± 9.3	$0.191 {\pm} 0.001$	0.230 ± 0.002
Neural-LP	115016.6 ± 0.0	0.070 ± 0.000	0.073 ± 0.000	90000.4 ± 0.0	0.238 ± 0.000	0.274 ± 0.000	21130.5 ± 0.0	0.170 ± 0.000	0.209 ± 0.000
DRUM	115016.6 ± 0.0	0.069 ± 0.001	0.073 ± 0.000	90000.3 ± 0.0	0.261 ± 0.000	0.274 ± 0.000	21130.5 ± 0.0	0.166 ± 0.001	0.209 ± 0.000
AnyBURL	108079.6 ± 0.0	0.096 ± 0.000	0.108 ± 0.000	83136.8 ± 5.3	0.191 ± 0.001	$0.252 {\pm} 0.001$	20530.8 ± 0.0	0.177 ± 0.000	0.214 ± 0.000
PTransE	111024.3 ± 855.0	0.069 ± 0.000	0.071 ± 0.000	86793.2 ± 961.0	0.249 ± 0.001	0.274 ± 0.000	18888.7 ± 457.3	0.158 ± 0.001	0.195 ± 0.002
RPJE	113082.0 ± 945.2	0.070 ± 0.000	0.072 ± 0.000	$89173.1 {\pm} 797.3$	0.267 ± 0.000	0.274 ± 0.000	20290.4 ± 417.2	$0.166{\pm0.001}$	0.206 ± 0.002
TransD	74277.3 ± 2907.8	0.052 ± 0.001	0.104 ± 0.002	52159.4 ± 758.9	0.238 ± 0.002	$0.280 {\pm} 0.003$	16698.1 ± 370.2	0.116 ± 0.004	0.189 ± 0.009
ANALOGY	$93383.4 {\pm} 20576.5$	0.072 ± 0.004	0.107 ± 0.002	60161.5 ± 3295.5	0.286 ± 0.004	0.318 ± 0.001	$18880.0 {\pm} 1213.8$	0.150 ± 0.005	0.211 ± 0.005
QuatE	$145603.8 {\pm} 1114.4$	0.103 ± 0.001	0.114 ± 0.001	94684.4 ± 1781.7	0.101 ± 0.009	$0.209{\pm0.011}$	26485.0 ± 491.8	0.157 ± 0.003	0.179 ± 0.002
BiQUE	81687.5 ± 603.2	0.104 ± 0.000	0.115 ± 0.000	61015.2 ± 399.8	0.135 ± 0.002	$0.205 {\pm} 0.007$	19079.4 ± 389.7	0.163 ± 0.002	0.185 ± 0.002
BiVE-Q	$\textbf{18.7} \!\pm\! \textbf{1.2}$	$0.748 \!\pm\! 0.007$	$0.853 \!\pm\! 0.004$	33.1 ± 17.4	0.531 ± 0.106	0.683 ± 0.114	56.6 ± 10.2	0.315 ± 0.024	0.523 ± 0.034
BiVE-B	19.7 ± 1.9	$\underline{0.731{\pm}0.010}$	$\underline{0.837{\pm0.006}}$	27.9±2.4	$\overline{0.555\pm0.007}$	$\overline{0.718\pm0.007}$	4.7±0.2	0.644 ± 0.004	$\overline{0.914 \pm 0.005}$

Table 3: Results of Triplet Prediction. The best scores are boldfaced and the second best scores are underlined. Our models, BiVE-Q and BiVE-B, significantly outperform all other baseline methods in terms of all metrics on all datasets.

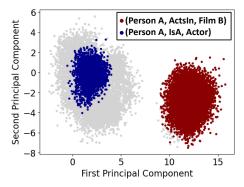


Figure 3: Embedding vectors of base-level triplets in $\langle T_i$, ImpliesProfession, $T_j \rangle$ where T_i is (Person A, ActsIn, Film B) and T_j is (Person A, IsA, Actor) in FBH. Both \mathbf{T}_i and \mathbf{T}_j embedding vectors from BiVE are well-clustered.

 $T_i = (h_i, r_i, t_i) \in \mathcal{E}_{train}$ denote a base-level triplet. We define $G_T := (\mathcal{E}_{\text{train}}, \widehat{\mathcal{R}}, \mathcal{H}_{\text{train}}),$ where each T_i is considered as an entity. If we train the baseline methods using G_T , the triplet prediction task can be considered as a link prediction problem on G_T . However, in this case, it is not guaranteed that all T_i involved in the triplets in \mathcal{H}_{test} appear in \mathcal{H}_{train} because we randomly split \mathcal{H} into training, validation, and test sets. Therefore, for the baseline methods, the problem becomes an inductive setting instead of a transductive setting. Indeed, among the baseline methods, Neural-LP and DRUM are inductive methods and we include these methods because they can conduct inductive inference. We assume that the candidates of a triplet prediction problem should be included in the training set of the base-level knowledge graph, which aligns with a realistic setting. By taking into account both the base-level knowledge graph and the higher-level triplets simultaneously, the problem becomes a transductive setting for BiVE. This shows that simply converting the higher-level triplets into G_T cannot replace

Table 3 shows the results of triplet prediction. We see that

BiVE-Q and BiVE-B significantly outperform all other stateof-the-art baseline methods in terms of all the three metrics on all three real-world datasets. Note that the number of candidates of a triplet prediction problem is equal to the number of base-level triplets in \mathcal{E}_{train} . Therefore, achieving the MR of 18.7 on FBH, for example, is surprising because we have 248,095 candidates in \mathcal{E}_{train} . We visualize the embedding vectors generated by BiVE-Q on FBH in Figure 3. We take all higher-level triplets in the form of $\langle T_i, \text{ImpliesProfession}, T_i \rangle$ and visualize the embedding vectors of T_i and T_j using Principal Component Analysis. In Figure 3, we only highlight the base-level triplets T_i and T_j where T_i is (Person A, ActsIn, Film B) and T_i is (Person A, IsA, Actor). We see that both T_i and T_i embedding vectors are well-clustered, meaning that BiVE generates embeddings by appropriately reflecting the structure of the higher-level triplets.

Conditional Link Prediction

To solve a conditional link prediction problem, BiVE uses the scoring function $F_{clp}(x)$. On the other hand, the baseline methods cannot directly solve the conditional link prediction problem. To allow the baseline methods to solve $\langle T_i, \hat{r}, (h_i, r_i, ?) \rangle^3$, we define a scoring function of the baseline methods as follows: $F(x) := f(\mathbf{h}_j, \mathbf{r}_j, \mathbf{x}) +$ $f(\mathbf{T}_i, \widehat{\mathbf{r}}, z(h_i, r_i, x))$ for all $x \in \mathcal{V}$ where the former is computed on the original base-level knowledge graph, the latter is computed on G_T , $z(h_i, r_i, x)$ returns an embedding vector of (h_i, r_i, x) , and $f(\cdot)$ is the scoring function of each baseline method. We cannot get $f(\mathbf{T}_i, \widehat{\mathbf{r}}, z(h_i, r_i, x))$ if $(h_i, r_i, x) \notin$ $\mathcal{E}_{\text{train}}$. In that case, we compute the score using the randomly initialized vectors in PTransE, RPJE, TransD, ANALOGY, QuatE, and BiQUE, whereas we set $f(\mathbf{T}_i, \hat{\mathbf{r}}, z(h_i, r_i, x)) = 0$ for the other baseline methods by considering the mechanisms of how each of the baseline methods assigns scores. In Table 4, BiVE-Q and BiVE-B significantly outperform all other

³We consider all four problems by changing the position of ?.

		FBH			FBHE			DBHE	
	$MR(\downarrow)$	MRR (†)	Hit@10 (†)	MR (↓)	MRR (†)	Hit@10 (†)	MR (↓)	MRR (†)	Hit@10 (†)
ASER	1183.9 ± 0.0	0.251 ± 0.000	0.316 ± 0.000	970.7 ± 0.0	0.289 ± 0.000	0.382 ± 0.000	1893.5 ± 0.0	0.225 ± 0.000	0.348 ± 0.000
MINERVA	3817.8 ± 58.9	0.328 ± 0.013	0.415 ± 0.009	3018.5 ± 45.8	0.407 ± 0.013	0.492 ± 0.014	2934.1 ± 32.2	0.362 ± 0.007	0.433 ± 0.014
Multi-Hop	1878.2 ± 12.0	0.421 ± 0.003	0.578 ± 0.003	1447.3 ± 11.9	0.443 ± 0.002	0.615 ± 0.002	1012.3 ± 28.5	0.442 ± 0.007	0.652 ± 0.008
Neural-LP	185.9 ± 1.3	0.433 ± 0.002	0.648 ± 0.004	146.2 ± 1.0	$0.466 {\pm} 0.002$	0.716 ± 0.007	32.2 ± 1.9	0.517 ± 0.006	0.756 ± 0.004
DRUM	262.7 ± 13.3	0.394 ± 0.002	0.555 ± 0.003	207.6 ± 10.0	0.413 ± 0.010	0.620 ± 0.018	49.0 ± 3.9	0.470 ± 0.010	0.732 ± 0.012
AnyBURL	228.5 ± 11.8	0.380 ± 0.004	0.563 ± 0.013	166.0 ± 7.9	0.418 ± 0.002	0.607 ± 0.008	81.7 ± 4.0	0.403 ± 0.002	0.594 ± 0.004
PTransE	214.8 ± 0.7	0.440 ± 0.001	0.686 ± 0.002	167.0 ± 1.8	0.516 ± 0.001	0.752 ± 0.001	19.3 ± 0.2	0.505 ± 0.004	0.780 ± 0.001
RPJE	212.5 ± 0.1	0.440 ± 0.001	0.686 ± 0.001	159.0 ± 0.0	0.528 ± 0.001	0.753 ± 0.001	19.3 ± 0.1	0.504 ± 0.004	0.779 ± 0.002
TransD	190.1 ± 18.0	0.300 ± 0.003	0.496 ± 0.005	165.6 ± 8.0	0.363 ± 0.003	0.529 ± 0.006	35.5 ± 1.0	0.436 ± 0.006	0.708 ± 0.005
ANALOGY	341.0 ± 218.7	0.182 ± 0.065	0.291 ± 0.125	113.3 ± 2.0	0.409 ± 0.004	0.581 ± 0.004	279.1 ± 197.1	0.140 ± 0.089	0.253 ± 0.166
QuatE	163.7 ± 3.6	0.346 ± 0.006	0.494 ± 0.011	1546.4 ± 98.0	0.124 ± 0.022	0.189 ± 0.014	551.6 ± 40.5	0.208 ± 0.013	0.309 ± 0.023
BiQUE	111.0 ± 0.9	0.423 ± 0.002	0.641 ± 0.002	90.1 ± 0.5	0.387 ± 0.009	0.617 ± 0.011	29.5 ± 1.2	0.378 ± 0.007	0.677 ± 0.004
BiVE-Q	7.0 ± 0.3	0.752 ± 0.005	0.906 ± 0.002	$11.0{\pm}0.3$	0.698 ± 0.004	$0.839 \!\pm\! 0.003$	12.5 ± 1.0	0.606 ± 0.009	0.828 ± 0.010
BiVE-B	6.6 ± 0.3	$\overline{0.762 \pm 0.007}$	$\overline{0.911\pm0.002}$	12.8 ± 0.4	$\underline{0.696{\pm0.005}}$	$\underline{0.834{\pm0.002}}$	3.2 ± 0.1	$\overline{0.801 \pm 0.003}$	0.958 ± 0.002

Table 4: Results of Conditional Link Prediction. The best scores are boldfaced and the second best scores are underlined. Our models, BiVE-Q and BiVE-B, significantly outperform all baseline methods in terms of all metrics on all datasets.

Problem	Prediction by BiVE-Q
\(\langle (?, \text{HasAFriendshipWith, Kelly_Preston}), \text{EquivalentTo, (Kelly_Preston, HasAFriendshipWith, George_Clooney)}\) \(\langle (?, \text{HasAFriendshipWith, Kelly_Preston}), \text{EquivalentTo, (Kelly_Preston, HasAFriendshipWith, Tom_Cruise)}\)	George_Clooney Tom_Cruise
((Joe Jonas, IsA, ?), ImpliesProfession, (Joe Jonas, IsA, Actor)) ((Joe Jonas, IsA, ?), ImpliesProfession, (Joe Jonas, IsA, Musician))	Voice_Actor Singer-songwriter
((Bucknell_University, HasAHeadquarterIn, Pennsylvania), ImpliesLocation, (?, Contains, Bucknell_University)) ((Bucknell_University, HasAHeadquarterIn, United_States), ImpliesLocation, (?, Contains, Bucknell_University))	Pennsylvania United_States
\(\lambda\)(\(\text{Saturn_Award_for_Best_Director, Nominates, Avatar)}\), \(\text{PrerequisiteFor, (Avatar, Wins, ?)}\)\)\(\lambda\)(\(\text{Academy_Award_for_Best_Visual_Effects, Nominates, Avatar)}\), \(\text{PrerequisiteFor, (Avatar, Wins, ?)}\)\)	Saturn_Award_for_Best_Director Academy_Award_for_Best_Visual_Effects

Table 5: Examples of Conditional Link Prediction on FBHE. BiVE correctly predicts the answers for all the above problems.

	FB	HE	DB	HE
	MR (↓)	Hit@10 (†)	MR (↓)	Hit@10 (†)
ASER	1489.3 ± 0.0	0.323 ± 0.000	2218.8 ± 0.0	0.197 ± 0.000
MINERVA	3828.4 ± 56.9	0.339 ± 0.003	3530.7 ± 50.1	0.297 ± 0.006
Multi-Hop	2284.0 ± 9.5	0.500 ± 0.001	2489.4 ± 15.3	0.404 ± 0.004
Neural-LP	1942.5 ± 0.5	0.486 ± 0.001	2904.8 ± 0.6	0.357 ± 0.001
DRUM	1945.6 ± 0.8	0.490 ± 0.002	2904.7 ± 0.7	0.359 ± 0.001
AnyBURL	342.0 ± 4.6	0.526 ± 0.002	879.1 ± 5.7	0.364 ± 0.003
PTransE	2077.6 ± 10.3	0.333 ± 0.000	3346.0 ± 20.0	0.277 ± 0.002
RPJE	1754.6 ± 7.5	0.368 ± 0.001	2991.7 ± 28.1	0.341 ± 0.000
TransD	166.3 ± 1.3	0.527 ± 0.001	429.0 ± 7.5	0.423 ± 0.001
ANALOGY	227.3 ± 8.3	0.486 ± 0.002	621.5 ± 20.9	0.323 ± 0.008
QuatE	139.0 ± 1.6	0.581 ± 0.001	409.6 ± 8.5	0.440 ± 0.001
BiQUE	134.9 ± 0.9	0.583 ± 0.001	376.6 ± 3.5	0.446 ± 0.002
BiVE-Q	125.2 ± 0.9	0.584 ± 0.001	405.4 ± 4.1	0.438 ± 0.002
BiVE-B	$\overline{123.5 \pm 1.0}$	0.586 ± 0.001	377.3 ± 6.7	0.444 ± 0.001

Table 6: Results of Base-Level Link Prediction.

baseline methods in conditional link prediction on all three real-world datasets. In Table 5, we show some example problems of conditional link prediction in *FBHE* and the predictions made by BiVE-Q where it correctly predicts the answers. When we consider a problem in the form of $\langle T_i, \hat{r}, (h_j, r_j, ?) \rangle$, even though we have the same problem of $(h_j, r_j, ?)$, the answer becomes different depending on T_i . This is the difference between the typical base-level link prediction and the conditional link prediction.

Base-Level Link Prediction

We present the performance of the typical base-level link prediction in Table 6. Since the base-level knowledge graphs of FBH and FBHE are identical, the performance of all baseline methods is the same on FBH and FBHE. The base-level link prediction performance of BiVE on FBH and FBHE is also very similar to each other. We observed that the MRR scores of our BiVE models and the two best baselines are almost the same on FBHE and DBHE. On FBHE, the average MRR scores of BiVE-Q and QuatE are both 0.354, and those of BiVE-B and BiQUE are both 0.356. On DBHE, the average MRR score of BiVE-Q is 0.265 and that of QuatE is 0.264; the average MRR score of BiVE-B is 0.275 and that of BiQUE is 0.274. Overall, our BiVE models show comparable results to the baseline methods for the typical link prediction task; our BiVE models have the extra capability of dealing with the triplet prediction and conditional link prediction tasks.

Data Augmentation of BiVE

We analyze the augmented triplets that are added by our data augmentation strategy. In Table 7, we show some examples of a relation sequence p_k , a relation r, and the confidence of (p_k, r) , the number of augmented triplets based on (p_k, r) denoted by $|\mathcal{S}_{kr}|$, and examples of the augmented triplets in FBHE and DBHE. According to our random walk policy, we

	Relation Sequence p_k	Relation r	$c(p_k, r)$	$ S_{kr} $	Examples of the Augmented Triplets
	NominatesIn, NominatesIn ⁻¹ , ActsIn, ImpliesProfession , IsA	IsA	0.86	610	(Patty_Duke, IsA, Actor)
	ParticipatesIn, ParticipatesIn ⁻¹ , ImpliesSports , Plays ⁻¹ , ParticipatesIn	ParticipatesIn	0.81	57	(Houston_Rockets, ParticipatesIn, 2003_NBA_Draft)
FBHE	Plays, Plays ⁻¹ , ImpliesSports ⁻¹ , HasPosition	HasPosition	0.78	295	(Bayer_04_Leverkusen, HasPosition, Forward)
	Contains, Contains ⁻¹ , ImpliesLocation ⁻¹ , HasAHeadquarterIn	Contains	0.72	81	(United_States, Contains, Charlottesville_Virginia)
	Program ⁻¹ , Program, Language	Language	0.70	148	(David_Copperfield_(Film), Language, English_Language)
	Genre, ImpliesGenre ⁻¹ , Genre, Genre ⁻¹ , ImpliesGenre ⁻¹ , Genre	Genre	0.78	120	(Kenny_Rogers, Genre, Pop_Rock)
	IsPartOf, IsPartOf, ImpliesLocation, IsPartOf	IsPartOf	0.76	69	(San_Pedro_Los_Angeles, IsPartOf, California)
DBHE	IsPartOf, IsPartOf ⁻¹ , ImpliesLocation ⁻¹ , IsPartOf ⁻¹ , TimeZone	TimeZone	0.75	122	(Brockton_Massachusetts, TimeZone, Eastern_Time_Zone)
	IsProducedBy ⁻¹ , IsProducedBy, ImpliesProfession , IsA	IsA	0.73	80	(Jim_Wilson, IsA, Film_Producer)
	Region, Region ⁻¹ , Country	Country	0.70	41	(Pontefract, Country, England)

Table 7: Examples of the Augmented Triplets in FBHE and DBHE. The higher-level relations are boldfaced.

	FBH	FBHE	DBHE
No. of unique (p_k, r)	340,194	349,120	149,365
No. of (p_k, r) with $c(p_k, r) \ge 0.7$	35,803	39,727	7,030
No. of augmented triplets	16,601	17,463	2,026
$ \mathcal{S} \cap \mathcal{E}_{ ext{valid}} + \mathcal{S} \cap \mathcal{E}_{ ext{test}} $	5,237	5,380	316

Table 8: Statistics of the Augmented Triplets.

		FBH	FBHE	DBHE
TP	$L_{\mathrm{base}} + L_{\mathrm{high}}$	19.2	28.1	65.4
	$L_{\text{base}} + L_{\text{high}} + L_{\text{aug}}$	18.7	33.1	56.6
CLP	$L_{\text{base}} + L_{\text{high}}$	8.3	12.5	12.4
CLI	$L_{\text{base}} + L_{\text{high}} + L_{\text{aug}}$	7.0	11.0	12.5
	L_{base}	139.0	139.0	409.6
BLP	$L_{ m base} + L_{ m high}$	138.4	138.4	408.1
BLP	$L_{\mathrm{base}} + L_{\mathrm{aug}}$	124.7	125.2	404.9
	$L_{\mathrm{base}} + L_{\mathrm{high}} + L_{\mathrm{aug}}$	124.7	125.2	405.4

Table 9: Ablation study of BiVE with different combinations of the loss terms. The average MR scores on triplet prediction (TP), conditional link prediction (CLP), and the base-level link prediction (BLP).

do not allow going back to an entity that has already been visited. Thus, even though a relation and its reverse relation are consecutively appeared in a relation sequence in Table 7, it does not mean that we return back to the previous entity; instead, it means that the walk steps another entity adjacent to the corresponding relation. In Table 8, we show statistics of the augmented triplets. Among the diverse combinations of a relation sequence p_k and a relation r, we consider the (p_k, r) pairs whose confidence scores are greater than or equal to 0.7. It is interesting to see that there exist considerable overlaps between the set $\mathcal S$ of the augmented triplets and $\mathcal E_{\text{valid}}$ and $\mathcal E_{\text{test}}$, indicating that our augmented triplets include many ground-truth triplets that are missing in the training set.

Ablation Study of BiVE

In BiVE, we have three different types of loss terms: $L_{\rm base}$, $L_{\rm high}$, and $L_{\rm aug}$. Using different combinations of these loss terms, we measure the performance of BiVE to check the importance of each loss term. Table 9 shows the average MR scores of BiVE-Q with different combinations of the loss

		Tri	plet Pred	iction	Conditional LP			
\widehat{r}	Freq.	MR	MRR	Hit@10	MR	MRR	Hit@10	
EquivalentTo	98	17.5	0.416	0.679	2.2	0.744	0.977	
ImpliesLanguage	29	35.6	0.292	0.578	18.4	0.632	0.786	
ImpliesProfession	210	71.3	0.427	0.569	11.5	0.704	0.844	
ImpliesLocation	163	42.2	0.219	0.463	9.4	0.502	0.816	
ImpliesTimeZone	44	20.6	0.354	0.631	17.8	0.604	0.707	
ImpliesGenre	84	113.8	0.177	0.345	32.6	0.408	0.681	
NextAlmaMater	14	71.0	0.161	0.379	2.5	0.651	0.971	
TransfersTo	29	67.0	0.140	0.374	5.7	0.527	0.537	

Table 10: Performance of BiVE per higher-level relation in DBHE. Freq. indicates the number of higher-level triplets in $\mathcal{H}_{\text{test}}$ associated with \hat{r} .

terms in three tasks: triplet prediction (TP), conditional link prediction (CLP), and base-level link prediction (BLP). Note that TP and CLP require at least two terms, $L_{\rm base}$ and $L_{\rm high}$. Also, Table 10 shows the performance of BiVE-Q per higher-level relation in DBHE, where Freq. indicates the number of higher-level triplets in $\mathcal{H}_{\rm test}$ associated with \widehat{r} . Among the eight higher-level relations in DBHE, NextAlmaMater and TransfersTo require externally-sourced knowledge. While EquivalentTo is the easiest one, the performance on the other higher-level relations varies depending on the tasks and the metrics.

Conclusion

We define a bi-level knowledge graph by introducing the higher-level relationships between triplets. We propose BiVE, which takes into account the structures of the base-level triplets, the higher-level triplets, and the augmented triplets. Experimental results show that BiVE significantly outperforms state-of-the-art methods in terms of the two newly defined tasks: triplet prediction and conditional link prediction. We believe our method can contribute to advancing many knowledge-based applications, including conditional QA [31] and multi-hop QA [8], with a special emphasis on mixing a neural language model and structured knowledge [38].

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Appendix

Experimental Settings

All experiments are conducted on machines equipped with Intel(R) Xeon(R) E5-2690 v4 CPUs and 512GB memory. We use RTX A6000 GPUs unless otherwise stated.

Baseline Methods

In experiments, we use 12 different baseline methods which are ASER [39], MINERVA [6], Multi-Hop [22], Neural-LP [37], DRUM [29], AnyBURL [25], PTransE [23], RPJE [27], TransD [15], ANALOGY [24], QuatE [40], and BiQUE [11]. We use GeForce RTX 2080Ti GPUs to run MINERVA, Neural-LP, and DRUM because these methods use TensorFlow version 1.

For ASER, we implement the string matching based inference model described in [39]. The original program of MINERVA is designed only to predict a tail entity. We add reversed triplets to also predict a head entity. In Multi-Hop, we set all the add_reverse_edge options to be true. We run AnyBURL with different rule learning times: 10 seconds, 100 seconds, 1,000 seconds and 10,000 seconds. Since the results of running 10,000 seconds are similar to those of 1,000 seconds, we use the results of 1,000 seconds. We use the best hyperparameters provided by the authors of each of the baseline methods except PTransE, RPJE, TransD, ANALOGY, QuatE, and BiQUE; we tune the hyperparameters of PTransE, RPJE, TransD, ANALOGY, QuatE, and BiQUE because the best hyperparameters are not provided for these methods.

For PTransE and RPJE, we tune the learning rate α using the range of $\alpha=\{10^{-6},5\cdot10^{-6},10^{-5},5\cdot10^{-5},10^{-4},5\cdot10^{-4}\}$ and the margin γ using the range of $\gamma=\{0.5,1.0,2.0\}$. We use TransD, ANALOGY, QuatE, and BiQUE, which are implemented based on OpenKE [13]. For TransD, we tune the learning rate α using the range of $\alpha=\{0.1,0.5,1.0,2.0,5.0\}$ and the margin γ using the range of $\gamma=\{2.0,5.0,10.0\}$. For ANALOGY, we tune the learning rate α using the range of $\alpha=\{0.001,0.005,0.01,0.05,0.1,0.05\}$ and the regularization rate β using the range of $\beta=\{0.5,1.0,2.0\}$. For QuatE and BiQUE, we tune the learning rate α using the range of $\alpha=\{0.1,0.5,1.0,2.0,5.0\}$ and the regularization rate β using the range of $\beta=\{0.1,0.5,1.0\}$. For TransD, ANALOGY, QuatE, and BiQUE, validation is done every 50 epochs up to 500 epochs, and we select the best epoch based on the validation results. Table 11 shows the best hyperparameters of these methods for the triplet prediction and the base-level link prediction. For the conditional link prediction problem, we combine the scores of the triplet prediction and the base-level link prediction as described in the main paper; we use the best hyperparameters of the triplet prediction and the base-level link prediction.

		Triplet Prediction	Base-Level Link Prediction
PTransE	FBH	$\alpha = 5 \cdot 10^{-6}, \gamma = 0.5$	$\alpha = 10^{-6}, \gamma = 0.5$
	FBHE	$\alpha = 5 \cdot 10^{-6}, \gamma = 0.5$	$\alpha = 10^{-6}, \gamma = 0.5$
	DBHE	$\alpha = 10^{-6}, \gamma = 0.5$	$\alpha = 10^{-6}, \gamma = 0.5$
RPJE	FBH	$\alpha = 10^{-6}, \gamma = 1.0$	$\alpha = 10^{-6}, \gamma = 1.0$
	FBHE	$\alpha = 10^{-6}, \gamma = 1.0$	$\alpha = 10^{-6}, \gamma = 1.0$
	DBHE	$\alpha = 10^{-6}, \gamma = 1.0$	$\alpha = 10^{-6}, \gamma = 1.0$
TransD	FBH	$\alpha = 0.5, \gamma = 5.0$	$\alpha = 1.0, \gamma = 5.0$
	FBHE	$\alpha = 0.1, \gamma = 5.0$	$\alpha = 1.0, \gamma = 5.0$
	DBHE	$\alpha = 0.5, \gamma = 5.0$	$\alpha = 0.1, \gamma = 5.0$
ANALOGY	FBH	$\alpha = 0.5, \beta = 0.5$	$\alpha = 0.01, \beta = 0.5$
	FBHE	$\alpha = 0.001, \beta = 0.5$	$\alpha = 0.01, \beta = 0.5$
	DBHE	$\alpha = 0.5, \beta = 0.5$	$\alpha = 0.005, \beta = 1.0$
QuatE	FBH	$\alpha = 0.5, \beta = 0.1$	$\alpha = 0.1, \beta = 0.1$
	FBHE	$\alpha = 0.5, \beta = 0.1$	$\alpha = 0.1, \beta = 0.1$
	DBHE	$\alpha = 1.0, \beta = 0.1$	$\alpha = 0.5, \beta = 0.5$
BiQUE	FBH	$\alpha = 0.5, \beta = 0.1$	$\alpha = 0.1, \beta = 0.1$
	FBHE	$\alpha = 0.5, \beta = 0.1$	$\alpha = 0.5, \beta = 0.1$
	DBHE	$\alpha = 0.5, \beta = 0.5$	$\alpha = 0.5, \beta = 0.1$

Table 11: The best hyperparameters of PTransE, RPJE, TransD, ANALOGY, QuatE, and BiQUE. α, β, γ indicate the learning rate, the regularization rate, and the margin, respectively.

			FI	ВН			FB	HE			DB	HE	
		α	β	λ_1	λ_2	α	β	λ_1	λ_2	α	β	λ_1	λ_2
	Triplet Prediction	0.1	0.1	1.0	0.5	0.1	0.1	0.5	0.2	0.5	0.5	0.2	1.0
BiVE-Q Co	Conditional Link Prediction	0.1	0.1	1.0	1.0	0.1	0.1	1.0	0.5	0.5	0.5	1.0	0.5
	Base-Level Link Prediction	0.1	0.1	0.2	0.5	0.1	0.1	0.2	0.2	0.5	0.5	0.2	0.5
	Triplet Prediction	0.1	0.1	1.0	1.0	0.1	0.1	0.5	1.0	0.1	0.1	0.2	0.2
BiVE-B	Conditional Link Prediction	0.1	0.1	1.0	1.0	0.1	0.1	1.0	1.0	0.1	0.1	1.0	0.5
	Base-Level Link Prediction	0.1	0.1	0.2	0.2	0.1	0.1	0.5	0.2	0.5	0.5	0.2	0.2

Table 12: The best hyperparameters of BiVE on validation.

Hyperparameters of BiVE

Within BiVE, we use the scoring function of QuatE [40] for BiVE-Q and BiQUE [11] for BiVE-B. On the validation set, we tune the learning rate α , the regularization rate β , and the weights λ_1 and λ_2 in L_{BiVE} . We use the search space of $\{0.2, 0.5, 1.0\}$ for both λ_1 and λ_2 . Validation is done every 50 epochs up to 500 epochs, and we select the best epoch based on the validation results. Table 12 shows the best hyperparameters of BiVE on the validation sets.

Real-World Bi-Level Knowledge Graphs

We describe the details about how we create the three real-world bi-level knowledge graphs, FBH, FBHE, and DBHE.

Base-Level Knowledge Graphs

We use FB15K237 [32] as the base-level knowledge graphs for FBH and FBHE. FB15K237 is a standard benchmark knowledge graph dataset which is constructed by taking 401 most frequent relations and merging near-duplicate and inverse relations in FB15K [3] from Freebase [2].

We use a filtered version of *DB15K* [10] which is constructed based on *DBpedia* [1]. By following the strategy used in [36], we first remove the relations that are not in the form of *DBpedia* URL, such as 'http://www.w3.org/2000/01/rdf-schema#seeAlso', since these types of relations do not have clear semantics. Then, we take the relations involved in more than 100 triplets and merge near-duplicate and inverse relations by following the strategy used in [32]. For example, (Chevrolet, owningCompany, General_Motors) and (Chevrolet, owner, General_Motors) are merged.

Higher-Level Triplets

In Table 13, we show the higher-level relations and the corresponding examples of the higher-level triplets used to create *FBH*, *FBHE*, and *DBHE*. While *FBHE* contains all ten higher-level relations, *FBH* contains only the first six higher-level relations.

Among the higher-level relations in Table 13, WorksFor, SucceededBy, TransfersTo, and HigherThan in FBHE and NextAlmaMater and TransfersTo in DBHE require externally-sourced knowledge. For example, we crawled Wikipedia articles to find information about the (vice)presidents of the United States, the teams a player was playing for, and the alma mater of politicians. Also, to create $\langle T_i$, HigherThan, $T_j \rangle$ in FBHE, we used the most recent rankings of Fortune 1000 and Times University Ranking. Table 14 and Table 15 show all types of higher-level triplets used to create FBH, FBHE, and DBHE.

	\widehat{r}	$\langle T_i, \widehat{r}, T_j angle$	Description
	PrerequisiteFor	T_i : (BAFTA_Award, Nominates, The_King's_Speech) T_j : (The_King's_Speech, Wins, BAFTA_Award)	For The King's Speech to win BAFTA Award, BAFTA Award should nominate The King's Speech.
	EquivalentTo	T_i : [Hillary Clinton, IsMarried To, Bill Clinton] T_j : (Bill Clinton, IsMarried To, Hillary Clinton)	The two triplets indicate the same information.
	ImpliesLocation	T_i : (Sweden, CapitalIsLocatedIn, Stockholm) T_j : (Sweden, Contains, Stockholm)	'The capital of Sweden is Stockholm' implies 'Sweden contains Stockholm'.
FBHE .	ImpliesProfession	T _j : (Liam_Neeson, IsA, Actor)	'Liam Neeson acts in Love Actually' implies 'Liam Neeson is an actor'.
	ImpliesSports	$\overline{T_i}$: (Boston_Red_Socks, HasPosition, Infield) T_j : (Boston_Red_Socks, Plays, Baseball)	'Boston Red Socks has an infield position' implies 'Boston Red Socks plays baseball'.
	NextEventPlace	$T_i: \overline{(1932_Summer_Olympics, IsHeIdIn, Los_Angeles)}$ $T_j: \overline{(1936_Summer_Olympics, IsHeIdIn, Berlin)}$	Summer Olympics in 1932 and 1936 were held in Los Angeles and Berlin, respectively. 1936 Summer Olympics is the next event of 1932 Summer Olympics.
	WorksFor	$\overline{T_i}$: (Joe_Biden, HoldsPosition, Vice_President) T_j : (Barack_Obama, HoldsPosition, President)	Joe Biden was a vice president when Barack Obama was a president of the United States.
	SucceededBy	T_i : (George_WBush, HoldsPosition, President) T_j : (Barack_Obama, HoldsPosition, President)	President Barack Obama succeeded President George W. Bush.
	TransfersTo	$\overline{T_i}$: (David_Beckham, PlaysFor, Real_Madrid_CF) T_j : (David_Beckham, PlaysFor, LA_Galaxy)	David Beckham transferred from Real Madrid CF to LA Galaxy.
	HigherThan	T_i : (Walmart, IsRankedIn, Fortune_500) T_j : (Bank_of_America, IsRankedIn, Fortune_500)	Walmart is ranked higher than Bank of America in Fortune 500.
	EquivalentTo	T_i : [David_Beckham, IsMarriedTo, Victoria_Beckham) T_j : (Victoria_Beckham, IsMarriedTo, David_Beckham)	The two triplets indicate the same information.
	ImpliesLanguage	T_i : (Italy, HasOffficialLanguage, Italian_Language) T_j : (Italy, UsesLanguage, Italian_Language)	"The official language of Italy is the Italian language' implies 'The Italian language is used in Italy'.
	ImpliesProfession	1 j: (Alfred_Hitchcock, IsA, Film_Producer)	'Psycho is directed by Alfred Hitchcock' implies 'Alfred Hitchcock is a film producer'.
DBHE	ImpliesLocation	T_i : (Mariah Carey, LivesIn, New York City) T_j : (Mariah Carey, LivesIn, New York)	'Mariah Carey lives in New York City' implies 'Mariah Carey lives in New York'
DBIIL	ImpliesTimeZone	<i>I</i> _j : (Prague, TimeZone, Central_European)	"Czech Republic is included in Central European Time Zone" implies 'Prague is included in Central European Time Zone'.
	ImpliesGenre	T_i : (Pharrell_Williams, Genre, Progressive_Rock) T_j : (Pharrell_Williams, Genre, Rock_Music)	"Pharrell Williams is a progressive rock musician' implies 'Pharrell Williams is a rock musician'.
	NextAlmaMater	$\overline{T_i}$: (Gerald Ford, Studies In, University of Michigan) T_j : (Gerald Ford, Studies In, Yale University)	Gerald Ford studied in University of Michigan. Then, he studied in Yale University.
	TransfersTo	T_i : (Ronaldo, PlaysFor, FC_Barcelona) T_j : (Ronaldo, PlaysFor, Inter_Millan)	Ronaldo transferred from FC Barcelona to Inter Millan.

Table 13: The higher-level relations and the corresponding examples of the higher-level triplets used to create *FBHE*, and *DBHE*.

		Example	Frequency	
	T_i : (Person A, DatesWith, Person B)	(Bruce_Willis, DatesWith, Demi_Moore)	222	
	T_i : (Person A, BreaksUpWith, Person B)	(Bruce_Willis, BreaksUpWith, Demi_Moore)		
(T. D T.)	T _i : (Award A, Nominates, Work B)	(BAFTA_Award, Nominates, The_King's_Speech)	2.225	
$\langle T_i, \text{PrerequisiteFor}, T_j \rangle$	T_i : (Work B, Wins, Award A)	(The_King's_Speech, Wins, BAFTA_Award)	2,335	
	T _i : (Person A, HasNationality, Country B)	(Neymar, HasNationality, Brazil)	109	
	T_i : (Person A, PlaysFor, National Team of B)	(Neymar, PlaysFor, Brazil_National_Football_Team)	109	
	T _i : (Person A, IsASibling To, Person B)	(Serena_Williams, IsASiblingTo, Venus_Williams)		
	T_i : (Person B, IsASiblingTo, Person A)	(Venus_Williams, IsASiblingTo, Serena_Williams)	120	
	T _i : (Person A, IsMarriedTo, Person B)	(Hillary-Clinton, IsMarriedTo, Bill-Clinton)		
(T_i : (Person B, IsMarriedTo, Person A)	(Bill_Clinton, IsMarriedTo, Hillary_Clinton)	352	
$\langle T_i, \text{EquivalentTo}, T_j \rangle$	T_i : (Person A, HasAFriendshipWith, Person B)	(Bob_Dylan, HasAFriendshipWith, The_Beatles)		
	T_i : (Person B, HasAFriendshipWith, Person A)	(The_Beatles, HasAFriendshipWith, Bob_Dylan)	1,832	
	T_i : (Person A, IsAPeerOf, Person B)	(Jimi_Hendrix, IsAPeerOf, Eric_Clapton)		
	T_i : (Person B, IsAPeerOf, Person A)	(Eric_Clapton, IsAPeerOf, Jimi_Hendrix)	132	
	T_i : (Location A, Contains, Location B)	(England, Contains, Warwickshire)	 2,415	
	T_i : (Location containing A, Contains, Location in B)	(United_Kingdom, Contains, Birmingham)		
	T_i : (Organization A, Headquarter, Location B)	(Kyoto-University, Headquarter, Kyoto)		
$\langle T_i, \text{ImpliesLocation}, T_j \rangle$	T_i : (Cocation B, Contains, Organization A)	(Kyoto, Contains, Kyoto-University)	820	
	T_j : (Country A, CapitalIsLocatedIn, City B)	(Sweden, CapitalIsLocatedIn, Stockholm)		
	T_i : (Country A, Capitaris Docated III, City B)	(Sweden, Contains, Stockholm)	83	
	T_j : (County A, Contains, City B) T_i : (Person A, IsA, Specialized Profession of B)	(Mariah-Carey, IsA, Singer-songwriter)		
	T_i : (Person A, IsA, Specialized Profession of B) T_i : (Person A, IsA, Profession B)	(Mariah-Carey, IsA, Musician)	2,364	
	T_j : (Rock&Roll Hall of Fame, Inducts, Person A)	(Narian-Carey, IsA, Musician) (Rock&Roll_Hall_of_Fame, Inducts, Bob_Dylan)		
	T_i : (Rock&Roll Hall of Fallie, finducts, Person A) T_i : (Person A, IsA, Musician/Artist)	(Bob_Dylan, IsA, Musician)	66	
	T_j : (Film A, IsWrittenBy, Person B)	(127_Hours, IsWrittenBy, Danny_Boyle)		
$\langle T_i, \text{ImpliesProfession}, T_i \rangle$			893	
	T_j : (Person B, IsA, Writer/Film Producer)	(Danny_Boyle, IsA, Film_producer)		
	T_i : (Person A, ActsIn, Film B)	(Liam_Neeson, ActsIn, Love_Actually)	10,864	
	T_j : (Person A, IsA, Actor)	(Liam_Neeson, IsA, Actor)		
	T _i : (Person A, HoldsPosition, Government Position B)	(Barack_Obama, HoldsPosition, President)	120	
	T_j : (Person A, IsA, Politician)	(Barack_Obama, IsA, Politician)		
	T_i : (Team A, HasPosition, Position of B)	(Boston_Red_Socks, HasPosition, Infield)	2,936	
	T_j : (Team A, Plays, Sports B)	(Boston_Red_Socks, Plays, Baseball)		
$\langle T_i, \text{ImpliesSports}, T_i \rangle$	$\overline{T_i}$: (League of A, Includes, Team B)	(National_League, Includes, New_York_Mets)	824	
(11, impliessports, 13)	T_j : (Team B, Plays, Sports A)	(New_York_Mets, Plays, Baseball)		
	$\overline{T_i}$: (Team A, ParticipatesIn, Draft of B)	(Atlanta_Braves, ParticipatesIn, MLB_Draft)	528	
	T_j : (Team A, Plays, Sports B)	(Atlanta_Braves, Plays, Baseball)	340	
$\langle T_i, \text{NextEventPlace}, T_i \rangle$	T _i : (Event A, IsHeldIn, Location A)	(1932_Summer_Olympics, IsHeldIn, Los_Angeles)	47	
(11, NextEventi face, 11)	T_j : (Next Event of A, IsHeldIn, Location B)	(1936_Summer_Olympics, IsHeldIn, Berlin)	47	
$\langle T_i, \text{WorksFor}, T_i \rangle$	T _i : (Person A, HoldsPosition, Vice President)	(Joe_Biden, HoldsPosition, Vice_President)	13	
$\langle T_i, \text{WorksPoi}, T_j \rangle$	T_j : (Person B, HoldsPosition, President)	(Barack_Obama, HoldsPosition, President)	13	
$\langle T_i, \text{SucceededBy}, T_i \rangle$	T _i : (Person A, HoldsPosition, President/Vice President)	(George_WBush, HoldsPosition, President)	30	
$\langle I_i, \text{Succeeded by}, I_j \rangle$	T_i : (Person B, HoldsPosition, President/Vice President)	(Barack_Obama, HoldsPosition, President)	30	
$\langle T_i, \text{TransfersTo}, T_i \rangle$	T _i : (Person A, PlaysFor, Team B)	(David_Beckham, PlaysFor, Real_Madrid_CF)	277	
$\langle I_i, \text{ Transfers 10}, I_j \rangle$	T _i : (Person A, PlaysFor, Team C)	(David_Beckham, PlaysFor, LA_Galaxy)	377	
/T. HistoryTheory (T.)	T _i : (Item A, IsRankedIn, Ranking List C)	(Walmart, IsRankedIn, Fortune_500)	7.450	
$\langle T_i, HigherThan, T_j \rangle$	T _i : (Item B, IsRankedIn, Ranking List C)	(Bank_of_America, IsRankedIn, Fortune_500)	7,459	

Table 14: All types of higher-level triplets to create FBH and FBHE.

		Example	Frequency
	T _i : (Person A, IsMarriedTo, Person B)	(Hillary_Clinton, IsMarriedTo, Bill_Clinton)	314
	T_j : (Person B, IsMarriedTo, Person A)	(Bill_Clinton, IsMarriedTo, Hillary_Clinton)	314
$\langle T_i, \text{EquivalentTo}, T_i \rangle$	T _i : (Location A, UsesLanguage, Language B)	(Brazil, UsesLanguage, Portuguese_Language)	120
(1 _i , Equivalent 10, 1 _j)	T_j : (Language B, IsSpokenIn, Location A)	(Portuguese_Language, IsSpokenIn, Brazil)	
	$\overline{T_i}$: (Person A, Influences, Person B)	(Baruch_Spinoza, Influences, Immanuel_Kant)	394
	T_j : (Person B, IsInfluencedBy, Person A)	(Immanuel_Kant, IsInfluencedBy, Baruch_Spinoza)	
	T _i : (Location A, HasOfficialLanguage, Language B)	(Italy, HasOfficialLanguage, Italian_Language)	196
T_i , ImpliesLanguage, T_j	T _j : (Location A, UsesLanguage, Language B)	(Italy, UsesLanguage, Italian_Language)	
- i, gg-, - j /	$\overline{T_i}$: (Location A, UsesLanguage, Language B)	(United_States, UsesLanguage, English_Language)	75
	T _j : (Location in A, UsesLanguage, Language B)	(California, UsesLanguage, English-Language)	
	T _i : (Work A, MusicComposedBy, Person B)	(Forrest_Gump, MusicComposedBy, Alan_Silvestri)	553
	T _j : (Person B, IsA, Musician/Composer)	(Alan_Silvestri, IsA, Composer)	
	T _i : (Work A, Starring, Person B)	(Love_Actually, Starring, Liam_Neeson)	737
	T_j : (Person B, IsA, Actor)	(Liam_Neeson, IsA, Actor)	
	T _i : (Work A, CinematographyBy, Person B)	(Jurassic_Park, CinematographyBy, Dean_Cundey)	299
T_i , ImpliesProfession, T_i	T_j : (Person B, IsA, Cinematographer) T_i : (Work A, IsDirectedBy, Person B)	(Dean_Cundey, IsA, Cinematographer) (Psycho, IsDirectedBy, Alfred_Hitchcock)	
•	T_i : (Work A, IsDirected By, Person B) T_i : (Person B, IsA, Film_Director/Television_Director)	(Alfred_Hitchcock, IsA, Film_Director)	295
	T_i : (Work A, IsProducedBy, Person B)	(King_Kong, IsProducedBy, Merian_CCooper)	
	T_i : (Work A, Isl Toduccuby, Ferson B) T_i : (Person B, IsA, Film_Producer/Television_Producer)	(Merian_CCooper, IsA, Film_Producer)	354
	T_i : (Person A, Associates With Record Label, Record B)	(Bo_Diddley, AssociatesWithRecordLabel, Atlantic_Records)	155
	T_i : (Person A, IsA, Record_Producer)	(Bo_Diddley, IsA, Record_Producer)	
	T_i : (Location A, IsPartOf, Location B)	(Ann_Arbor, IsPartOf, Washtenaw_County_Michigan)	
	T_i : (Location in A, IsPartOf, Location Containing B)	(Ann_Arbor, IsPartOf, Michigan)	1,174
	T_i : (Organization A, IsLocatedIn, Location B)	(Adobe_Systems, IsLocatedIn, San_Jose_California)	250
$\langle T_i, \text{ImpliesLocation}, T_j \rangle$	T_i : (Organization A, IsLocatedIn, Location Containing B)	(Adobe_Systems, IsLocatedIn, California)	
	T_i : (Person A, LivesIn, Location B)	(Mariah_Carey, LivesIn, New_York_City)	
	T_i : (Person A, LivesIn, Location Containing B)	(Mariah_Carey, LivesIn, New_York)	213
	T_i : (Location A, TimeZone, Time Zone B)	(Czech_Republic, TimeZone, Central_European_Time)	
$\langle T_i, \text{ImpliesTimeZone}, T_j \rangle$	T_i : (Location in A, TimeZone, Time Zone B)	(Prague, TimeZone, Central_European_Time)	409
	T _i : (Musician A, Genre, Genre B)	(Pharrell_Williams, Genre, Progressive_Rock)	
$\langle T_i, \text{ImpliesGenre}, T_j \rangle$	T_i : (Musician A, Genre, Parent Genre of B)	(Pharrell_Williams, Genre, Rock_Music)	767
//// Nit Alma Matan ///	T_i : (Person A, StudiesIn, Institution B)	(Gerald Ford, StudiesIn, University of Michigan)	
$\langle T_i, \text{NextAlmaMater}, T_j \rangle$	T_i : (Person A, StudiesIn, Institution C)	(Gerald_Ford, StudiesIn, Yale_University)	112
- $ -$	T _i : (Person A, PlaysFor, Team B)	(Ronaldo, PlaysFor, FC_Barcelona)	
$\langle I_i, \text{ transfers to, } I_j \rangle$	T_i : (Person A, PlaysFor, Team C)	(Ronaldo, PlaysFor, Inter_Millan)	300

Table 15: All types of higher-level triplets to create *DBHE*.