Box Embeddings for the Description Logic $\mathcal{EL}^{++}$

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Abstract

Recently, various methods for representation learning on Knowledge Bases (KBs) have been developed. However, these approaches either only focus on learning the embeddings of the data-level knowledge (ABox) or exhibit inherent limitations when dealing with the concept-level knowledge (TBox), e.g., not properly modelling the structure of the logical knowledge. We present BoxEL, a geometric KB embedding approach that allows for better capturing logical structure expressed in the theories of Description Logic $\mathcal{EL}^{++}$. BoxEL models concepts in a KB as axis-parallel boxes exhibiting the advantage of intersectional closure, entities as points inside boxes, and relations between concepts/entities as affine transformations. We show theoretical guarantees (soundness) of BoxEL for preserving logical structure. Namely, the trained model of BoxEL embedding with loss 0 is a (logical) model of the KB. Experimental results on subsumption reasonings and a real-world application–protein-protein prediction show that BoxEL outperforms traditional knowledge graph embedding methods as well as state-of-the-art $\mathcal{EL}^{++}$ embedding approaches.

1 Introduction

Knowledge Bases (KBs) provide a conceptualization of objects and their relationships, which are useful in applications like biomedical and intelligent systems (Rector, Rogers, and Pole, 1996; Consortium, 2015). Such KBs are often expressed using Description Logics (DLs) (Baader et al., 2003), a family of languages allowing for expressing domain knowledge via logical statements (a.k.a axioms). These logical statements are divided into two parts: 1) an ABox consisting of assertions over instances, i.e., factual statements, such as John is the father of Peter, written as isFatherOf(John, Peter); 2) a TBox consisting of logical statements constraining concepts, e.g., Parent $\subseteq$ Person meaning that Parent is a subclass of Person.

KBs not only provide clear semantics in the application domains but also enable (classic) reasoners (Steigmiller, Liebig, and Glimm, 2014; Kazakov, Krötzsch, and Simancik, 2014) to perform logical inference, i.e., making implicit knowledge explicit. Existing reasoners are highly optimized and scalable but they are limited to only computing classical logical entailment, i.e., they are not designed to perform inductive/analogical reasoning and to handle noisy data. Embedding based methods, which map the objects in the KBs into a low dimensional vector space while keeping the similarity for analogical reasoning, have been proposed to complement the classical reasoners and shown remarkable performance gains in various applications.

Most KB embeddings methods (Wang et al., 2017) focus on embedding data-level knowledge in ABoxes, a.k.a., Knowledge Graph Embeddings (KGEs). Although effective, KGEs cannot preserve the concept-level knowledge (the logical structure expressed in TBoxes). Recently, embedding based methods for KBs expressed in DLs have been explored, prominent examples include $\mathcal{EL}^{++}$ (Kulmanov et al., 2019) that supports conjunction and full existential quantification, and $\mathcal{AC}C$ (Özçep, Leemhuis, and Wolter, 2020) that further supports logical negation. We focus on $\mathcal{EL}^{++}$, an underlying formalism of the OWL2 EL profile of the Web Ontology Language (Grau et al., 2008) that has been used in expressing various biomedical ontologies (Consortium, 2015; Rector, Rogers, and Pole, 1996).

In order to learn embeddings of $\mathcal{EL}^{++}$ KBs, several approaches such as Onto2Vec (Smaili, Gao, and Hoehndorf, 2018), OWL2Vec (Chen et al., 2021) and OPA2Vec (Smaili, Gao, and Hoehndorf, 2019) have been proposed. These approaches require annotation data and cannot model logical structure explicitly. Geometric representations, in which the objects are associated with geometric objects such as balls (Kulmanov et al., 2019) and convex cones (Özçep, Leemhuis, and Wolter, 2020), provide a high expressiveness.

Figure 1: Two counterexamples of Ball embedding and its relational transformation. (a) Ball embedding cannot express concept equivalence Parent $\cap$ Male $\equiv$ Father with intersection operator. (b) The translation cannot model relation (e.g. isChildOf) between Person and Parent when they should have different volumes. These two issues can be solved by Box embedding and modeling relation as affine transformation, respectively.
on embedding logical properties. For $\mathcal{EL}^{++}$ KBs, ELEm (Kulmanov et al., 2019) represents concepts as open $n$-balls and relations as a translation. ELEm preserves some of the logical structure and has been shown to outperform classical KGEs. Although effective, ELEm, which uses ball embeddings, still suffers from several major limitations:

- Balls are not closed under intersection, which limits capturing common logic structures. For example, the intersection of two concepts $\text{Parent} \cap \text{Male}$, that is supposed to represent $\text{Father}$, is not a ball (see Fig. 1(a)). Therefore, the concept equivalence $\text{Parent} \cap \text{Male} \equiv \text{Father}$ cannot be captured in the embedding space.

- Simple translation as used in TransE suffers from various limitations (Wang et al., 2014). This causes further issues for concept embeddings when want to model the size of concepts. For example, Fig. 1(b) illustrates the embeddings of the axiom $\exists \text{ChildOf. Person} \sqsubseteq \text{Parent}$ assuming the existence of another axiom $\text{Parent} \sqsubseteq \text{Person}$. In this case, it is impossible to translate the larger concept $\text{Person}$ into the smaller one $\text{Parent}$, as it does not allow for scaling the size.

- ELEm does not distinguish between entities in ABox and concepts in TBox, but rather regards ABox axioms as special cases of TBox axioms. Such simplification cannot fully express the logical structure well in the KB, e.g., an entity must have minimal volume.

To overcome these limitations, we consider modeling concepts in the KB as boxes (i.e., axis-aligned hyperrectangles), encoding entities as points inside the boxes that they should belong to, and the relations as the affine transformation between boxes and/or points. Fig. 1(a) shows that the box embedding with closed form of intersection and the affine transformation (Fig. 1(b)) can naturally capture the cases that are not possible in ELEm. In this way, we present BoxEL for embedding KBs expressed by DL $\mathcal{EL}^{++}$, in which the interpretation functions of $\mathcal{EL}^{++}$ theories in the KB can be represented by the geometric transformations between boxes/points. We formulate BoxEL as an optimization task by designing and minimizing various loss terms between boxes and/or points. Fig. 1(a) shows that we use a different encoding that distinguishes between entities and concepts. Furthermore, we take advantage of affine transformation that have various inherent advantages as discussed before. Another difference of our method is that we use a different encoding that distinguishes between entities and concepts. Moreover, we take advantage of the volume of boxes (instead of the distance) for disjointedness representation, leading to a more natural encoding of the disjointedness of concepts, i.e., two concepts are disjoint iff their intersection box has zero volume.

2 Related Work

In this section, we review some related works on KB embeddings, including classical knowledge graph embeddings, as well as concept embeddings with logical descriptions.

2.1 Knowledge Graph Embeddings

Knowledge graph embeddings (KGEs) have been developed for different tasks. Early works, which focus on link prediction, embed both entities and relations as vectors in a vector space to model the relationships between entities (Bordes et al., 2013; Trouillon et al., 2016; Dettmers et al., 2018). Prominent examples include additive (or translational) family (Bordes et al., 2013; Wang et al., 2014; Lin et al., 2015) and multiplicative (or bilinear) family (Nickel, Tresp, and Kriegel, 2011; Yang et al., 2015; Liu, Wu, and Yang, 2017). Such techniques only embed the data-level part of KBs and work relatively well for the link prediction tasks. However, KGEs demonstrate limitations when being used to learn the representation of background knowledge such as ontologies of logical rules (Garg et al., 2019; Özçep, Leemhuis, and Wolter, 2020), as well as complex logic expressions (Ren, Hu, and Leskovec, 2020; Ren and Leskovec, 2020).

2.2 Concept Embeddings

Recently, several methods have been proposed to embed concepts to regions in vector spaces including balls (Kulmanov et al., 2019; Mondal, Bhatia, and Mutharaju, 2021) and convex cones (Özçep, Leemhuis, and Wolter, 2020). For query answering, entities are mapped to points and queries are embedded to boxes (Ren, Hu, and Leskovec, 2020) such that the answers of a given query are included inside the corresponding box for that query. Such geometric methods nicely model set theory that can be used to capture logical rules of KGs (Aboud et al., 2020) and to represent transitive closure relations (e.g. WordNet) (Vilnis et al., 2018).

Among embeddings for complex concept descriptions, boxes have some conceptual advantages, but they have not been exploited for representing ontologies yet. Other works such as quantum embedding (Sun et al., 2020) captures expressive DLs like $\mathcal{ALC}$ KBs consisting of a large ABox and a small TBox. In contrast, our approach focuses on $\mathcal{EL}^{++}$ that has a larger TBox. Our work is closely related to ELEm (Kulmanov et al., 2019), but instead of using ball embedding and translation, we consider box embedding and affine transformation that have various inherent advantages as discussed before. Another difference of our method is that we use a different encoding that distinguishes between entities and concepts. Furthermore, we take advantage of the volume of boxes (instead of the distance) for disjointedness representation, leading to a more natural encoding of the disjointedness of concepts, i.e., two concepts are disjoint iff their intersection box has zero volume.

3 Description Logic $\mathcal{EL}^{++}$

We consider the DL $\mathcal{EL}^{++}$ that underlies multiple biomedical KBs like GALEN (Rector, Rogers, and Pole, 1996) and the Gene Ontology (Consortium, 2015). Formally, the syntax of $\mathcal{EL}^{++}$ is built up from a set $N_I$ of individual names, $N_C$ of concept names and $N_R$ of role names (also called relations) using the constructors shown in Table 1, where $N_I$, $N_C$ and $N_R$ are pairwise disjoint. Strictly speaking, $\mathcal{EL}^{++}$ also allows for concrete domains, but we do not make use of them here.
The semantics of $\mathcal{EL}^{++}$ is defined by interpretations $I = (\Delta^T, \mathcal{I})$, where the domain $\Delta^T$ is a non-empty set and $\mathcal{I}$ is a mapping that associates every individual with an element in $\Delta^T$, every concept name with a subset of $\Delta^T$, and every relation name with a relation over $\Delta^T \times \Delta^T$. An interpretation is satisfied if it satisfies the corresponding semantic conditions. The syntax and the corresponding semantics (i.e., interpretation of concept expressions) of $\mathcal{EL}^{++}$ are summarized in Table 1.

| Constructors | Syntax | Semantics |
|--------------|--------|-----------|
| Top concept  | $\top$ | $\Delta^T$ |
| Bottom concept | $\bot$ | $\emptyset$ |
| Nominal      | $\{a\}$ | $\{a\} \subseteq \Delta^T$ |
| Conjunction  | $C \sqcap D$ | $C \cap D \subseteq \Delta^T$ |
| Existential restriction | $\exists r.C$ | $\{ x \in \Delta^T \mid \exists y \in \Delta^T (x,y) \in r \land y \in C \}$ |
| ABox Concept inclusion | $C(a)$ | $a \in C \subseteq \Delta^T$ |
| ABox Role assertion | $r(a,b)$ | $a^r \in C^2 \subseteq \Delta^T \times \Delta^T$ |
| TBox Concept inclusion | $C$ | $C \subseteq \Delta^T$ |

| ABox | Concept assertion | Role assertion |
|------|------------------|----------------|
| $C(a)$ | $a \in C \subseteq \Delta^T$ | $a^r \in C^2 \subseteq \Delta^T \times \Delta^T$ |

Conceptually, we understand points as boxes of volume 0. This will be helpful later to encode the meaning of axioms for points and boxes in a uniform way. Intuitively, $m_w : N_I \cup N_C \rightarrow \mathbb{R}^n$ maps individual and concept names to the lower left corner and $M_w : N_I \cup N_C \rightarrow \mathbb{R}^n$ maps them to the upper right corner of the box that represents them. For individuals $a \in N_I$, we have $m_w(a) = M_w(A)$, so that it is sufficient to store only one of them. The box associated with $C$ is defined as

$$\text{Box}_w(C) = \{ x \in \mathbb{R}^n \mid m_w(C) \leq x \leq M_w(C) \},$$

where the inequality is defined component-wise.

Note that boxes are closed under intersection, which allows us to compute the volume of the intersection of boxes. The lower corner of the (possibly empty) box $\text{Box}_w(C) \cap \text{Box}_w(D)$ is $\min(m_w(C), m_w(D))$ and the upper corner is $\max(M_w(C), M_w(D))$, where minimum and maximum are taken component-wise. The volume of boxes can be used to encode axioms in a very concise way. However, as we will see later, one problem is that points have volume 0. This does not allow distinguishing empty boxes from points. To show that our encoding correctly captures the logical meaning of axioms, we will consider a modified volume that assigns a non-zero volume to points and some empty boxes. The (modified) volume of a box is defined as

$$M\text{Vol}(\text{Box}_w(C)) = \prod_{i=1}^n \max(0, M_w(C)_i - m_w(C)_i + \epsilon),$$

where $\epsilon > 0$ is a small constant. A point now has volume $\epsilon^n$. Some empty boxes can actually have arbitrarily large modified volume. For example the 2D-box with lower corner $(0,0)$ and upper corner $(-\frac{\epsilon}{2}, N)$ has volume $\epsilon \frac{N}{2}$. While this is not meaningful geometrically, it does not cause any problems for our encoding because we only want to ensure that boxes with volume 0 are empty (and not points).

We associate every role name $r \in N_R$ with an affine transformation denoted by $T_w^r(x) = D_w^r x + b_w^r$, where $D_w^r$ is an $(n \times n)$ diagonal matrix with non-negative entries and $b_w^r \in \mathbb{R}^n$ is a vector. In a special case where all diagonal entries of $D_w^r$ are 1, $T_w^r(x)$ captures translations. Note that relations have been represented by translation vectors analogous to TransE in (Kulmanov et al., 2019). However, this necessarily means that the concept associated with the range of a role has the same size as its domain. This does not seem very intuitive, in particular, for N-to-one relationships like has_nationality or lives_in that map many objects to the same object. Note that our approach Note that $T_w^r(\text{Box}_w(C)) = \{ T_w^r(x) \mid x \in \text{Box}_w(C) \}$ is the box with lower corner $m_w(C)_i = T_w^r(M_w(C))$. To show this, note that $m_w(C) < M_w(C)$ implies $D_w m_w(C) \leq D_w M_w(C)$ because $D_w$ is a diagonal matrix with non-negative entries. Hence, $T_w^r(M_w(C)) = D_w^r m_w(C) + b_w^r \leq D_w^r M_w(C) + b_w^r = T_w^r(M_w(C))$. For $m_w(C) \geq M_w(C)$, both $\text{Box}_w(C)$ and $T_w^r(\text{Box}_w(C))$ are empty.

Overall, we have the following parameters:

- for every individual name $a \in N_I$, we have $n$ parameters for the vector $m_w(a)$ (since $m_w(a) = M_w(A)$, we have...
to store only one of $m_w$ and $M_w$).

- for every concept name $C \in N_C$, we have $2n$ parameters for the vectors $m_w(C)$ and $M_w(C)$,
- for every role name $r \in N_r$, we have $2n$ parameters, $n$ parameters for the diagonal elements of $D^r_w$ and $n$ parameters for the components of $b^r_w$.

As we explained informally before, $w$ summarizes all parameters. The overall number of parameters in $w$ is $n \cdot (|N_I| + 2 \cdot |N_C| + 2 \cdot |N_r|)$.

4.2 Geometric Interpretation

The next step is to encode the axioms in our KB. However, we do not want to do this in an arbitrary fashion, but, ideally, in a way that gives us some analytical guarantees. (Kulmanov et al., 2019) made an interesting first step in this direction by showing that their encoding is sound. In order to understand soundness, it is important to know that the parameters of the embedding are learnt by minimizing a loss function that contains a loss term for every axiom. Soundness then means that if the loss function yields 0, then the KB is satisfiable. Recall that satisfiability means that there is an interpretation that satisfies all axioms in the KB. Ideally, we should be able to construct such an interpretation directly from our embedding. This is indeed what the authors in (Kulmanov et al., 2019) did. The idea is that points in the vector space map up the domain of the interpretation, the points that lie in regions associated with concepts correspond to the interpretation of this concept and the interpretation of roles correspond to translations between points like in TransE. In our context, such a geometric interpretation can be defined as follows.

**Definition 1** (Geometric Interpretation). Given a parameter vector $w$ representing an $\mathcal{EL}^{++}$ embedding, the corresponding geometric interpretation $I_w = (\Delta^w, \tau_w)$ is defined as follows:

1. $\Delta^w = \mathbb{R}^n$,
2. for every concept name $C \in N_C$, $C^w = Box_w(C)$,
3. for every role $r \in N_r$, $r^w = \{(x, y) \in \Delta^w \times \Delta^w \mid \tau^w_r(x) = y\}$,
4. for every individual name $a \in N_I$, $a^w = m_w(a)$.

We will now encode the axioms by defining one loss term for every axiom that can occur in a normalized $\mathcal{EL}^{++}$ KB. The design principle of each loss term is to guarantee that the axiom is satisfied by the geometric interpretation when the loss term is 0.

4.3 ABox Embedding

ABox contains concept assertions and role assertions. We introduce the following two loss terms that respect the geometric interpretations.

**Concept Assertion** Geometrically, a concept assertion $C(a)$ asserts that the point $m_w(a)$ is inside the box $Box_w(C)$ (see Fig. 2(a)). This can be expressed by demanding $m_w(C) \leq m_w(a) \leq M_w(C)$ for every component. The loss term $L_{C(a)}(w)$ is defined by

$$L_{C(a)}(w) = \sum_{i=1}^{n} \|\max(0, m_w(a)_i - M_w(C)_i)\|_2 + \sum_{i=1}^{n} \|\max(0, m_w(C)_i - m_w(a)_i)\|_2.$$  \hspace{1cm} (3)

**Role Assertion** Geometrically, a role assertion $r(a, b)$ means that the point $m_w(a)$ should be mapped to $m_w(b)$ by the transformation $T^r_r$ (see Fig. 2(b)). That is, we should have $T^r_r(m_w(a)) = m_w(b)$. We define a the loss term via

$$L_{r(a, b)}(w) = \|T^r_r(m_w(a)) - m_w(b)\|_2.$$  \hspace{1cm} (4)

It is clear from the definition that when the loss terms are 0, the axioms are satisfied in their geometric interpretation.

**Proposition 1.** We have

1. If $L_{C(a)}(w) = 0$, then $I_w \models C(a)$.
2. If $L_{r(a, b)}(w) = 0$, then $I_w \models r(a, b)$.

Proposition 1 follows immediately from the definitions.

4.4 TBox Embedding

For the TBox, we define loss terms for the four cases in the normalized KB. Before doing so, we define an auxiliary function that will be helpful for several axioms.

**Definition 2** (Disjoint measurement). Given two boxes $B_1, B_2$, the disjoint measurement can be defined by the (modified) volumes of $B_1$ and the intersection box $B_1 \cap B_2$, given by

$$\text{Disjoint}(B_1, B_2) = 1 - \frac{MVol(B_1 \cap B_2)}{MVol(B_1)}.$$  \hspace{1cm} (5)

We have the following guarantees.

**Lemma 1.** 1. $0 \leq \text{Disjoint}(B_1, B_2) \leq 1$,
2. $\text{Disjoint}(B_1, B_2) = 0$ implies $B_1 \subseteq B_2$,
3. $\text{Disjoint}(B_1, B_2) = 1$ implies $B_1 \cap B_2 = \emptyset$. 
Proof. 1. Since $B_1 \cap B_2 \subseteq B_1$, \allowbreak \allowbreak \frac{\text{MVol}(B_1 \cap B_2)}{\text{MVol}(B_1)} \leq 1$. The modified volume is also non-negative, so that the fraction is non-negative and $0 \leq \text{Disjoint}(B_1, B_2) \leq 1$.

2. If \text{Disjoint}(B_1, B_2) = 0 then we must have \text{MVol}(B_1 \cap B_2) = 1 and therefore \text{MVol}(B_1 \cap B_2) = \text{MVol}(B_1) \neq 0. Since $B_1 \cap B_2 \subseteq B_1$, this is only possible if $B_1 \cap B_2 = B_1$, but this implies that $B_1 \cap B_2 = B_2$.

3. If \text{Disjoint}(B_1, B_2) = 1, we must have \text{MVol}(B_1 \cap B_2) = 0. By definition of the modified volume this is only possible if $B_1 \cap B_2 = \emptyset$.

NF1: Atomic Subsumption An axiom of the form $C \subseteq D$ geometrically means that $\text{Box}_w(C) \subseteq \text{Box}_w(D)$ (see Fig. 2(c)). If $D \not\subseteq \bot$, we consider the loss term

$$L_{C \subseteq D}(w) = \text{Disjoint}(\text{Box}_w(C), \text{Box}_w(D)). \quad (6)$$

For the case that $D = \bot$ and $C$ is not a nominal, that is, $C \subseteq \bot$, we define the loss term

$$L_{C \subseteq \bot}(w) = \max(0, \text{MVol}(C) - m_w(C) + \epsilon). \quad (7)$$

If $C$ is a nominal, the axiom is inconsistent and our implementation can just return an error.

Proposition 2. If $L_{C \subseteq D}(w) = 0$, then $I_w \models C \subseteq D$, where we exclude the inconsistent case $C = \{a\}$, $D = \bot$.

Proof. For $D \not\subseteq \bot$, the claim follows from Lemma 1. For $D = \bot$, $L_{C \subseteq \bot}(w) = 0$ implies that $\text{Box}_w(C) = \emptyset$ and the claim is trivially true.

NF2: Conjunct Subsumption An axiom of the form $C \cap D \subseteq E$ means that $\text{Box}(C) \cap \text{Box}(D) \subseteq \text{Box}(E)$ (see Fig. 2(d)). Since $\text{Box}(C) \cap \text{Box}(D)$ is a box again, we can use the same idea as for NF1. For the case $E \not\subseteq \bot$, we define the loss term as

$$L_{C \cap D \subseteq E}(w) = \text{Disjoint}(\text{Box}_w(C) \cap \text{Box}_w(D), \text{Box}_w(E)). \quad (8)$$

For $E = \bot$, the axiom states that $C$ and $D$ must be disjoint. If the volume of the intersection of the associated boxes is 0, they must be disjoint (see Fig. 2(e)). However, just using the volume as a loss term may not work well because a minimization algorithm may minimize the volume of the boxes instead of the volume of their intersections. Therefore, we normalize the loss term by dividing by the volume of the boxes. Our loss term is

$$L_{C \cap D \subseteq \bot}(w) = \frac{\text{MVol}(\text{Box}_w(C) \cap \text{Box}_w(D))}{\text{MVol}(\text{Box}_w(D))}. \quad (9)$$

Proposition 3. If $L_{C \cap D \subseteq E}(w) = 0$, then $I_w \models C \cap D \subseteq E$, where we exclude the inconsistent case $a \cap a \subseteq \bot$ (that is, $C = D = \{a\}$, $E = \bot$).

Proof. We have to show that for every $x \in \text{Box}_w(C)$, there is a $y \in \text{Box}_w(D)$ such that $T_w^*(x) = y$. Note that $\text{Disjoint}(T_w^*(\text{Box}_w(C)), \text{Box}_w(D)) = 0$ implies that $T_w^*(\text{Box}_w(C)) \subseteq \text{Box}_w(D)$ according to Lemma 1. Since $x \in \text{Box}_w(C)$, we have $T_w^*(x) = y \in \text{Box}_w(D)$.

NF3: Right Existential Next, we consider axioms of the form $C \subseteq \exists r.D$. Note that $\exists r.D$ describes those entities that are in relation $r$ with an entity from $D$. Geometrically, those are points that are mapped to points in $\text{Box}_w(D)$ by the affine transformation corresponding to $r$. $C \subseteq \exists r.D$ then means that every point in $\text{Box}_w(C)$ must be mapped to a point in $\text{Box}_w(D)$, that is the mapping of $\text{Box}_w(C)$ is contained in $\text{Box}_w(D)$ (see Fig. 2(f)). Therefore, the encoding comes again down to encoding a subset relationship as before. The only difference to the first normal form is that $\text{Box}_w(C)$ must be mapped by the affine transformation $T_w^*$. These considerations lead to the following loss term

$$L_{C \subseteq \exists r.D}(w) = \text{Disjoint}(T_w^*(\text{Box}_w(C)), \text{Box}_w(D)). \quad (10)$$

Proposition 4. If $L_{C \subseteq \exists r.D}(w) = 0$, then $I_w \models C \subseteq \exists r.D$.

The proof of Proposition 4 is analogous to the proof of Proposition 3.

NF4: Left Existential Axioms of the form $\exists r.C \subseteq D$ can be treated symmetrically to the previous case (see Fig. 2(f)). We only consider the case $D \not\subseteq \bot$ and define the loss term

$$L_{\exists r.C \subseteq D}(w) = \text{Disjoint}(T_w^{-r}(\text{Box}_w(C)), \text{Box}_w(D)). \quad (11)$$

where $T_w^{-r}$ is the inverse function of $T_w^r$ that is defined by $T_w^{-r}(x) = D_w^r x - D_w^r r_w$, where $D_w^r$ is obtained from $D_w^r$ by replacing all diagonal elements with their reciprocal. Strictly speaking, the inverse only exists if all diagonal entries of $D_w^r$ are non-zero. However, we assume that the entries that occur in a loss term of the form $L_{\exists r.C \subseteq D}(w)$ remain non-zero in practice when we learn them iteratively.

Proposition 5. If $L_{\exists r.C \subseteq D}(w) = 0$, then $I_w \models \exists r.C \subseteq D$.

Proof. We have to show that if $T_w^{-r}(x) = y$ and $y \in \text{Box}_w(C)$, then $x \in \text{Box}_w(D)$. Disjoint$(T_w^{-r}(\text{Box}_w(C)), \text{Box}_w(D)) = 0$ implies that $T_w^{-r}(\text{Box}_w(C)) \subseteq \text{Box}_w(D)$ according to Lemma 1. Since $y \in \text{Box}_w(C)$, we have $x = T_w^{-r}(y) \in \text{Box}_w(D)$.

4.5 Optimization

Softplus Approximation For optimization, while the computation of the volume of boxes is straightforward, using a precise hard volume is known to cause problems when learning the parameters using gradient descent algorithms, e.g. there is no training signal (gradient flow) when box embeddings that should overlap but become disjoint (Li et al., 2019; Patel et al., 2020; Dasgupta et al., 2020). To mitigate the problem, there are several soft versions of volume calculation such as softplus volume (Patel et al., 2020) and GumbelBox (Dasgupta et al., 2020). We approximate the volume of boxes by the softplus volume due to its simplicity.

$$\text{SVol}(\text{Box}_w(C)) = \prod_{i=1}^{n} \text{Softplus}_t(M_w(C)_i - m_w(C)_i) \quad (12)$$

where $t$ is a temperature parameter. The softplus function is defined as $\text{softplus}_t(x) = t \log(1 + e^{x/t})$, which can be regarded as a smoothed version of the ReLu function ($\max(0, x)$) used for calculating the volume of hard boxes. In practice, the softplus volume is used to replace the modified volume in Eq.(2) as it empirically resolves the same issue that point has zero volume. We also use softplus function for updating box embedding. Hence, the boxes can be ensured to be non-empty.
from negative samples for all NF3 in the paper, we find that in their thus enlarge the boxes. Also makes sure that points in the boxes are spread out and the boxes from becoming very small. The negative sampling help the boxes to find their proper volume, thus preventing the process of training. Note that our overall loss terms will function with gradient descent. Algorithm 1 summarizes the terms, and learn the embeddings by minimizing the loss one of the head or tail entity.

\[ \text{Regularization} \quad \lambda = \sum_{i=1}^{n} \max(0, M_{w}(C)_i - 1 + \epsilon) + \max(0, -M_{w}(C)_i - \epsilon) \]  

(13)

In practice, this also avoids numerical stability issues. For example, to minimize a loss term, a box that should have a fixed volume could become very slim, i.e. some side lengths be extremely large while others become extremely small.

\[ \text{Negative Sampling} \quad \text{In principle, the embeddings can be optimized without negatives. However, we empirically find that the embeddings will be highly overlapped without negative sampling. e.g. for role assertion } r(a, b), \text{a and } b \text{ will simply become the same point. Similar to standard KGE methods and (Kulmanov et al., 2019), we generate negative samples for the role assertion } r(a, b) \text{ by randomly replacing one of the head or tail entity.} \]

Finally, we sum up all the loss terms and regularization terms, and learn the embeddings by minimizing the loss function with gradient descent. Algorithm 1 summarizes the process of training. Note that our overall loss terms will help the boxes to find their proper volume, thus preventing the boxes from becoming very small. The negative sampling also makes sure that points in the boxes are spread out and thus enlarge the boxes.

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\[ \text{Algorithm 1 Algorithm for training BoxEL} \]

\textbf{Input:} A KB \((A, T)\), dimension \(d\), epochs \(e\), batch size \(b\), and positive constants \(\theta\) and \(\gamma\).

\textbf{Output:} Embeddings \((f_r, f_e, f_t)\)

1: //Normalizing TBox with \(\mathcal{E}L^+\) rules
2: \(T \leftarrow\) normalization(\(T\))
3: //Generating negative samples
4: //Embeddings initialization
5: \(f_r = \text{uniform}(0, 1)\)
6: \(f_e = \text{uniform}(0, 1)\)
7: \(f_t = \text{uniform}(-0.9, 1.1)\)
8: \(f_r = \text{uniform}(-0.1, 0.1)\)
9: for \(e \in\) epochs do
10: \(ax_r \leftarrow \text{sample}(A, b)\)
11: \(ax_t \leftarrow \text{sample}(T, b)\)
12: \(neg_r \leftarrow \text{sample}(A, b)\)
13: //Update embeddings with SGD
14: \(\text{loss} = \text{model}(ax_r, ax_t, neg_r)\)
15: \(\Delta\text{loss}\)
16: end for

\[ \text{Figure 3: Visualization of the learned BoxEL embeddings in the family domain ontology.} \]

\section{5 Empirical Evaluation}

We evaluate BoxEL on three settings: 1) a toy example of family domain; 2) a subsumption reasoning task in three biomedical ontologies; and 3) a link prediction task (protein-protein prediction) in a real-world biomedical KB.

\subsection{5.1 A Proof-of-concept Example}

We begin by first validating the model in modeling a toy ontology–family domain (Kulmanov et al., 2019), which is described by the following axioms:\footnote{Although (Kulmanov et al., 2019) mentioned that they generate negative samples for all NF3 in the paper, we find that in their implementation, they only used the NF3 cases that are generated from \(r(a, b)\), which is the same as ours.}

\begin{align*}
\text{Male} \sqsubseteq \text{Person} & \quad \text{Female} \sqsubseteq \text{Person} \\
\text{Father} \sqsubseteq \text{Male} & \quad \text{Mother} \sqsubseteq \text{Female} \\
\text{Father} \sqsubseteq \text{Parent} & \quad \text{Mother} \sqsubseteq \text{Parent} \\
\text{Male} \sqcap \text{Parent} \sqsubseteq \text{Father} & \quad \exists \text{hasChild(Person)} \sqsubseteq \text{Parent} \\
\text{Parent} \sqsubseteq \text{Person} & \quad \exists \text{hasChild(Person)} \sqsubseteq \text{Parent} \\
\text{Father(Alex)} & \quad \text{Father(Bob)} \\
\text{Mother(Marie)} & \quad \text{Mother(Alice)} \\
\end{align*}

We set the dimension to 2 to visualize the embeddings. Fig. 3 shows that the generated embeddings accurately encode all of the axioms. In particular, the embeddings of \(\text{Father} \text{ and } \text{Mother}\) align well with the conjunction \(\text{Parent}\sqcap\text{Male} \text{ and } \text{Parent}\sqcap\text{Female}\), respectively, which is impossible to be achieved by ELEm.

\subsection{5.2 Subsumption Reasoning}

We evaluate the effectiveness of BoxEL on subsumption reasoning because most of the reasoning tasks in ontologies (e.g. axiom entailment, concept satisfiability and ABox consistency) can be reduced to subsumption reasoning (Baader, Brandt, and Lutz, 2005). The problem is to predict whether a concept is subsumed by another one. For each subsumption pair \(C \sqsubseteq D\), the scoring function can be defined by

\[ P(C \sqsubseteq D) = 1 - \frac{\text{MVol}(\text{Box}(C) \cap \text{Box}(D))}{\text{MVol}(\text{Box}(C))}. \]  

(14)
Table 2: The ranking based measures of embedding models on testing set. * denotes the results from (Mondal, Bhatia, and Mutharaju, 2021).

| Dataset | Metric   | TransE* | TransH* | DistMult* | ELEM | EmEL++ | BoxEL (Ours) |
|---------|----------|---------|---------|-----------|------|--------|--------------|
| GO      | Hits@10  | 0.00    | 0.00    | 0.00      | 0.09 | 0.10   | 0.09         |
|         | Hits@100 | 0.00    | 0.00    | 0.00      | 0.16 | 0.22   | 0.24         |
|         | AUC      | 0.53    | 0.44    | 0.50      | 0.70 | 0.76   | 0.83         |
|         | Mean Rank| -       | -       | -         | 13719| 11050  | 8010         |
| GALEN   | Hits@10  | 0.00    | 0.00    | 0.00      | 0.07 | 0.10   | 0.12         |
|         | Hits@100 | 0.00    | 0.00    | 0.00      | 0.14 | 0.17   | 0.23         |
|         | AUC      | 0.54    | 0.48    | 0.51      | 0.64 | 0.65   | 0.89         |
|         | Mean Rank| -       | -       | -         | 8321 | 8407   | 2922         |
| ANATOMY | Hits@10  | 0.00    | 0.00    | 0.00      | 0.18 | 0.18   | 0.19         |
|         | Hits@100 | 0.01    | 0.00    | 0.00      | 0.38 | 0.40   | 0.43         |
|         | AUC      | 0.53    | 0.44    | 0.49      | 0.73 | 0.76   | 0.92         |
|         | Mean Rank| -       | -       | -         | 28564| 24421  | 8688         |

Table 3: Summary of classes, relations and axioms in different ontologies. NF, represents the $i^{th}$ normal form.

| Ontology | GO | GALEN | ANATOMY |
|----------|----|-------|---------|
| Classes  | 45895 | 24353 | 106363  |
| Relations| 9  | 1010  | 157     |
| NF1      | 85480| 28890 | 122142  |
| NF2      | 12131| 13595 | 2121    |
| NF3      | 20324| 28118 | 152289  |
| NF4      | 12129| 13597 | 2143    |
| Disjoint | 30 | 100   | 184     |

Table 4: The accuracies (for which the prediction is true if and only if the subclass box is exactly inside the superclass box) achieved by the embeddings in terms of geometric interpretation of the classes in various ontologies.

|         | ELEM | EmEL++ | BoxEL |
|---------|------|--------|-------|
| GO      | 0.250| 0.415  | 0.538 |
| GALEN   | 0.480| 0.345  | 0.663 |
| ANATOMY | 0.069| 0.215  | 0.453 |

While the subsumption reasoning does not need negatives, we add an additional regularization term for non-subsumption axiom. In particular, for each atomic subsumption axiom $C \subseteq D$, we generate a non-subsumption axiom $C \nsubseteq D'$ or $C' \nsubseteq D$ by randomly replacing one of the concepts $C$ and $D$. Note that this does not produce regular negative samples as the generated concepts pair does not have to be disjoint. Thus, the loss term for non-subsumption axiom cannot be simply defined by $L_{C \nsubseteq D'} = 1 - L_{C \subseteq D'}$. Instead, we define the loss term as $L_{C \nsubseteq D'} = \phi(1 - L_{C \subseteq D'})$ by multiplying a small positive constant $\phi$ that encourages splitting the non-subsumption concepts while does not encourage them to be disjoint. If $\phi = 1$, the loss would encourage the non-subsumption concepts to be disjoint. We empirically show that $\phi = 1$ produces worse performance as we do not want non-subsumption concepts to be disjoint.

**Dataset** We use three biomedical ontologies as our benchmark. 1) **Gene Ontology (GO)** (Harris et al., 2004) integrates the representation of genes and their functions across all species. 2) **GALEN** (Rector, Rogers, and Pole, 1996) is a clinical ontology. 3) **Anatomy** (Mungall et al., 2012) is an ontology that represents linkages of different phenotypes to genes. The statistical information of these datasets are summarized in Table 3. The subclass relations are split into training set (70%), validation set (20%) and testing set (10%), respectively.

**Evaluation protocol** Two strategies can be used to measure the effectiveness of the embeddings. 1) Ranking based measures rank the probability of $C$ subsumed by all concepts. We evaluate and report four ranking based measures. Hits@10, Hits@100 describe the fraction of true cases that appear in the first 10 and 100 test cases of the sorted rank list, respectively. Mean rank computes the arithmetic mean over all individual ranks (i.e. $MR = \frac{1}{|I|} \sum_{rank \in I} rank$, where rank is the individual rank), while AUC computes the area under the ROC curve. 2) Accuracy based measure is a stricter criterion, for which the prediction is true if and only if the subclass box is exactly inside the superclass box (even not allowing the subclass box slightly outside the superclass box). We use this measure as it evaluates the performance of embeddings on retaining the underlying characteristics of ontology in vector space. We only compare ELEM and EmEL++ as KGE baselines fail in this setting (KGEs cannot preserve the ontology).

**Implementation details** The ontology is normalized into standard normal forms, which comprise a set of axioms that can be used as the positive samples. Similar to previous works (Kulmanov et al., 2019), we perform normalization using the OWL APIs and the APIs offered by the jCer reasoner [18]. The hyperparameter for negative sampling is set to $\phi = 0.05$. For ELEM and EmEL++, the embedding size is searched from $n = [50, 100, 200]$ and margin parameter $\gamma = [-0.1, 0.1]$. Since box embedding has double the number of parameters of ELEM and EmEL++, the embedding size is searched from $n = [25, 50, 100]$ for BoxEL. All experiments are evaluated with 10 random seeds that influence the data splitting, batch sequence and weight initialization. Mean results are reported for numerical comparisons.

**Baselines** We compare the state-of-the-art $\mathcal{E}L^{++}$ embeddings (ELEM) (Kulmanov et al., 2019), the first geometric embeddings of $\mathcal{E}L^{++}$, as well as the extension EmEL++ (Mondal, Bhatia, and Mutharaju, 2021) that additionally considers the role inclusion and role chain embedding, as
of embedding models. We first observe that both ELEm and EmEL perform much better than the three standard KGEs (TransE, TransH, and DistMult) on all three datasets, especially on hits@k for which KGEs fail, showcasing the limitations of KGEs and the benefits of geometric embeddings on encoding logic structures. EmEL++ performs slightly better than ELEm on all three datasets. Overall, our model BoxEL outperforms ELEm and EmEL+++. In particular, we find that our model achieves competitive results on Hit@10 and slightly better results on Hit@100, while for Mean Rank and AUC, it achieves significant performance gains on all three datasets. Note that Mean Rank and AUC have theoretical advantages over hits@k because hits@k is sensitive to any model performance changes while Mean Rank and AUC reflect the average performance, demonstrating that BoxEL achieves better average performance. Table 4 shows the accuracies of different embeddings in terms of the geometric interpretation of the classes in various ontologies. It clearly demonstrates that BoxEL outperforms ELEm and EmEL+++ by a large margin, showcasing that BoxEL preserves the underlying ontology characteristics in vector space better than ELEm and EmEL+++ that use ball embeddings.

### 5.3 Protein-Protein Interactions

Following (Kulmanov et al., 2019), we evaluate BoxEL on modeling the protein-protein interactions (PPI).

**Dataset** We use a biomedical knowledge graph built by (Kulmanov et al., 2019) from Gene Ontology (TBox) and STRING database (ABox) to conduct this task. Gene Ontology contains information about the functions of proteins, while STRING database consists of the protein-protein interactions. We use the protein-protein interaction data of yeast and human organisms, respectively. For each pair of proteins \((P_1, P_2)\) that exists in STRING, we add a role assertion \(\text{interacts}(P_1, P_2)\). If protein \(P\) is associated with the function \(F\), we add a membership axiom \(\{P\} \subseteq \exists\text{hasFunction}F\). The membership assertion can be regarded as a special case of NF3, in which \(P\) is a point (i.e., zero-volume box). The interaction pairs of proteins are split into training (80%), testing (10%) and validation (10%) sets. To perform prediction for each protein pair \((P_1, P_2)\), we predict whether the role assertion \(\text{interacts}(P_1, P_2)\) holds. This can be measured by the scoring function given by Eq.(15).

\[
P(\text{interacts}(P_1, P_2)) = \left\| \mathbf{w}^{\text{interacts}}(m_w(P_1)) - m_w(P_2) \right\|^2_2.
\]  

where \(\mathbf{w}^{\text{interacts}}\) is the affine transformation function for relation \(\text{interacts}\). For each positive interaction pair \(\text{interacts}(P_1, P_2)\), we generate a corrupted interaction pair by randomly replacing one of the head and tail proteins in order to generate the negative samples.

## Table 5: Prediction performance on protein-protein interaction (yeast).

| Method      | Raw Hits@10 | Filtered Hits@10 | Raw Hits@100 | Filtered Hits@100 | Raw Mean Rank | Filtered Mean Rank | Raw AUC | Filtered AUC |
|-------------|-------------|------------------|--------------|-------------------|--------------|--------------------|---------|-------------|
| TransE      | 0.06        | 0.13             | 0.32         | 0.40              | 1125         | 1075               | 0.82    | 0.83        |
| SimResnik   | 0.09        | 0.17             | 0.38         | 0.48              | 758          | 707                | 0.86    | 0.87        |
| SimLin      | 0.08        | 0.15             | 0.33         | 0.41              | 875          | 825                | 0.8     | 0.85        |
| ELEm        | 0.08        | 0.17             | 0.44         | 0.62              | 451          | 394                | 0.92    | 0.93        |
| EmEL+++     | 0.08        | 0.16             | 0.45         | 0.63              | 451          | 397                | 0.9     | 0.91        |
| Onto2Vec    | 0.08        | 0.15             | 0.35         | 0.48              | 641          | 588                | 0.79    | 0.80        |
| OPA2Vec     | 0.06        | 0.13             | 0.39         | 0.58              | 523          | 467                | 0.87    | 0.88        |
| Node2Vec    | 0.07        | 0.15             | 0.36         | 0.46              | 589          | 522                | 0.87    | 0.88        |
| BoxEL (Ours)| **0.09**     | **0.20**         | **0.52**     | **0.73**          | **423**      | **379**            | **0.93**| **0.94**    |

## Table 6: Prediction performance on protein-protein interaction (human).

| Method      | Raw Hits@10 | Filtered Hits@10 | Raw Hits@100 | Filtered Hits@100 | Raw Mean Rank | Filtered Mean Rank | Raw AUC | Filtered AUC |
|-------------|-------------|------------------|--------------|-------------------|--------------|--------------------|---------|-------------|
| TransE      | 0.05        | 0.11             | 0.24         | 0.29              | 3960         | 3891               | 0.78    | 0.79        |
| SimResnik   | 0.05        | 0.09             | 0.25         | 0.30              | 1934         | 1864               | 0.88    | 0.89        |
| SimLin      | 0.04        | 0.08             | 0.20         | 0.23              | 2288         | 2219               | 0.86    | 0.87        |
| ELEm        | 0.01        | 0.02             | 0.22         | 0.26              | 1680         | 1638               | 0.90    | 0.90        |
| EmEL+++     | 0.01        | 0.03             | 0.23         | 0.26              | 1671         | 1638               | 0.90    | 0.91        |
| Onto2Vec    | 0.05        | 0.08             | 0.24         | 0.31              | 2435         | 2391               | 0.77    | 0.77        |
| OPA2Vec     | 0.03        | 0.07             | 0.23         | 0.26              | 1810         | 1768               | 0.86    | 0.88        |
| BoxEL (Ours)| **0.07**     | **0.10**         | **0.42**     | **0.63**          | **1574**     | **1530**           | **0.93**| **0.93**    |
Baselines  We consider ELEm (Kulmanov et al., 2019) and EmEL++ (Mondal, Bhatia, and Mutharaju, 2021) as our two major baselines as they have been shown to outperform the traditional KGEs. We also report the result of Onto2Vec (Smaili, Gao, and Hoehndorf, 2018) that treats logical axioms as a text corpus and OPA2Vec (Smaili, Gao, and Hoehndorf, 2019) that combines logical axioms with annotation properties. Besides, we report the results of two semantic similarity measures, Resnik’s similarity and Lin’s similarity in (Kulmanov et al., 2019), for which the similarity between proteins is computed based on their associations with gene ontology classes. Finally, we compare Node2Vec (Grover and Leskovec, 2016), a graph-based embedding methods. We report the hits@10, hits@100, mean rank and AUC (area under the ROC curve) as explained before for numerical comparison. Both raw ranking measures and filtered ranking measures that ignore the triples that are already known to be true are reported. All baseline results are taken from the standard benchmark developed by (Kulmanov et al., 2021).

Overall Results  Table 5 and Table 6 summarize the performance of protein-protein prediction in yeast and human organisms, respectively. We first observe that similarity based methods (SimResnik and SimLin) roughly outperform TransE, showcasing the limitation of classical knowledge graph embeddings. The geometric methods ELEm and EmEL++ fail on the hits@10 measures and does not show significant performance gains on the hits@100 measures in human dataset. However, ELEm and EmEL++ outperform TransE and similarity based methods on Mean Rank and AUC by a large marginal, especially for the Mean Rank, showcasing the expressiveness of geometric embeddings. Onto2Vec and OPA2Vec achieve relatively better results than TransE and similarity based methods, but cannot compete ELEm and EmEL++. We conjecture that this is due to the fact that they mostly consider annotation information but cannot encode the logical structure explicitly. Our method, BoxEL consistently outperforms all methods in hits@100, Mean Rank and AUC in both datasets, except the competitive results of hits@10, showcasing the better expressiveness of BoxEL.

5.4 Ablation Studies

Transformation vs Translation  To study the benefits of using the box for modeling concepts and the affine transformation for modeling relations (i.e., how much gain is contributed by box and how much gain is from affine transformation), we conduct an ablation study by comparing relation embeddings with affine transformation (AffineBoxEL) and translation (TransBoxEL) of box embeddings. The only difference of TransBox to the AffineBox is that TransBox does not associate a scaling factor for each relation. Table 7 clearly shows that TransBoxEL also performs better than EmEL++, showcasing the benefits of box modeling compared with ball modeling. While AffineBoxEL further improves TransBoxEL, demonstrating the advantages of affine transformation. Hence, both box modeling and transformation relation modeling are crucial for KB embeddings.

Entities as Points vs Boxes  As we mentioned before, distinguishing entities and concepts by identifying entities as points in the boxes of concepts has better theoretical properties. Here, we study how does this distinction influence performance. For this purpose, we explore eliminating the ABox axioms by replacing each individual with a singleton class and rewriting relation assertions r(a, b) and concept assertions C(a) as \{a\} ⊑ \exists r.\{b\} and \{a\} ⊑ C, respectively. In this case, we only have TBox embeddings and the entities are embedded as regular boxes. Table 8 shows that for hits@k, there is marginal significant improvement of point entity embedding over boxes entity embedding, however, point entity embedding consistently outperforms box entity embedding on Mean Rank and AUC, showcasing the benefits of distinguishing entities and concepts.

6 Conclusion

This paper proposes BoxEL, a geometric KB embedding method that explicitly models the logical structure expressed by the theories of \(\mathcal{EL}^{++}\). Different from the standard KGEs that simply ignore the analytical guarantees, BoxEL provides soundness guarantee for the underlying logical structure by incorporating background knowledge into machine learning tasks. Hence, offering a more reliable and logic-preserved fashion for KB reasoning. The empirical results further demonstrate that BoxEL outperforms previous KGEs and \(\mathcal{EL}^{++}\) embedding approaches on subsumption reasoning over three ontologies and predicting protein-protein interactions in a real-world biomedical KB.

For future work, we are planning to look into constraint-based optimization approaches to get stronger analytical guarantees at the expense of computational performance. Since the volume of boxes can naturally capture joint probabilistic distribution (Vilnis et al., 2018), our approach can also be naturally extended to the probabilistic description logic StatisticalEL (Peñaloza and Potyka, 2017) that allows making statements about statistical proportions in a population.

Table 7: The prediction performance of BoxEL with affine transformation (AffineBoxEL) and BoxEL with translation (TransBoxEL) on yeast protein-protein interaction.

| Method                  | Hits@10 Raw | Hits@10 Filtered | Hits@100 Raw | Hits@100 Filtered | Mean Rank Raw | Mean Rank Filtered | AUC Raw | AUC Filtered |
|-------------------------|-------------|------------------|--------------|-------------------|---------------|-------------------|--------|-------------|
| ELEm                    | 0.08        | 0.17             | 0.04         | 0.18              | 451           | 394               | 0.92   | 0.93        |
| EmEL++                  | 0.44        | 0.62             | 0.54         | 0.68              | 451           | 394               | 0.92   | 0.93        |
| Onto2Vec                | 0.44        | 0.62             | 0.54         | 0.68              | 451           | 394               | 0.92   | 0.93        |
| OPA2Vec                 | 0.08        | 0.17             | 0.04         | 0.18              | 451           | 394               | 0.92   | 0.93        |
| Mean Rank               | 0.44        | 0.62             | 0.54         | 0.68              | 451           | 394               | 0.92   | 0.93        |
| AUC                     | 0.92        | 0.93             | 0.93         | 0.93              | 451           | 394               | 0.92   | 0.93        |

Table 8: The prediction performance of BoxEL with point entity embedding and box entity embedding on yeast protein-protein interaction dataset.

| Method                  | Hits@10 Raw | Hits@10 Filtered | Hits@100 Raw | Hits@100 Filtered | Mean Rank Raw | Mean Rank Filtered | AUC Raw | AUC Filtered |
|-------------------------|-------------|------------------|--------------|-------------------|---------------|-------------------|--------|-------------|
| ELEm                    | 0.08        | 0.17             | 0.04         | 0.18              | 451           | 394               | 0.92   | 0.93        |
| EmEL++                  | 0.44        | 0.62             | 0.54         | 0.68              | 451           | 394               | 0.92   | 0.93        |
| Onto2Vec                | 0.44        | 0.62             | 0.54         | 0.68              | 451           | 394               | 0.92   | 0.93        |
| OPA2Vec                 | 0.08        | 0.17             | 0.04         | 0.18              | 451           | 394               | 0.92   | 0.93        |
| Mean Rank               | 0.44        | 0.62             | 0.54         | 0.68              | 451           | 394               | 0.92   | 0.93        |
| AUC                     | 0.92        | 0.93             | 0.93         | 0.93              | 451           | 394               | 0.92   | 0.93        |
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