Description Logic $\mathcal{EL}^{++}$ Embeddings with Intersectional Closure

Xi Peng, Zhenwei Tang, Maxat Kulmanov, Kexin Niu, Robert Hoehndorf*
Computer, Electrical and Mathematical Sciences & Engineering Division (CEMSE), Computational Bioscience Research Center (CBRC), King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia
{xi.peng, zhenwei.tang, maxat.kulmanov, kexin.niu, robert.hoehndor} @kaust.edu.sa

Abstract
Many ontologies, in particular in the biomedical domain, are based on the Description Logic $\mathcal{EL}^{++}$. Several efforts have been made to interpret and exploit $\mathcal{EL}^{++}$ ontologies by distributed representation learning. Specifically, concepts within $\mathcal{EL}^{++}$ theories have been represented as $n$-balls within an $n$-dimensional embedding space. However, the intersectional closure is not satisfied when using $n$-balls to represent concepts because the intersection of two $n$-balls is not an $n$-ball. This leads to challenges when measuring the distance between concepts and inferring equivalence between concepts. To this end, we developed $\text{ELBE}$ (Box Embedding) to learn Description Logic $\mathcal{EL}^{++}$ embeddings using axis-parallel boxes. We generate specially designed box-based geometric constraints from $\mathcal{EL}^{++}$ axioms for model training. Since the intersection of boxes remains as a box, the intersectional closure is satisfied. We report extensive experimental results on three datasets and present a case study to demonstrate the effectiveness of the proposed method.

1 Introduction
$\mathcal{EL}^{++}$ is a lightweight Description Logic that admits sound and complete reasoning in polynomial time and has been used to define the Web Ontology Language (OWL) 2 EL profile [Motik et al., 2009]. $\mathcal{EL}^{++}$ is of great value in real-world applications, and especially in the life sciences where a large number of ontologies have been developed [Smith et al., 2007] and the OWL 2 EL profile is widely used [Hoehndorf et al., 2011].

Statistical methods [Subramanian et al., 2005] and semantic similarity measures [Pesquita et al., 2009] have been developed and widely used to analyze ontologies as well as entities characterized with concepts in ontologies. Recent years have witnessed increasing interest in distributed representation learning in a variety of fields including natural language processing [Mikolov et al., 2013] and recommender systems [He et al., 2017]. This motivated efforts in understanding and exploiting the Description Logic $\mathcal{EL}^{++}$ through embeddings [Kulmanov et al., 2019; Mondala et al., 2021]. The embedding methods for $\mathcal{EL}^{++}$ consider concepts as $n$-balls in an $n$-dimensional embedding space. The rationality behind representing concepts as geometric regions rather than single points in the embedding space is twofold. First, logical operations within ontological axioms, such as subsumptions and intersections, require geometric operations on top of regional representations. Second, the semantics of $\mathcal{EL}^{++}$ interprets concepts as sets of entities, and these are naturally represented as regions in the embedding space. Therefore, geometric embeddings not only fully fulfill the need of embedding $\mathcal{EL}^{++}$ axioms but also establish a direct correspondence to the semantics of the $\mathcal{EL}^{++}$ Description Logic.

Although these embedding methods are effective and theoretically well-motivated due to the relation between geometric regions and interpretations of the axioms, a common key issue remains unsolved: the intersectional closure, i.e., the property that the intersection of two concepts is again a concept within the embedding space, is not satisfied. Intuitively, the intersection of concept Parent and concept Male should also be a concept (i.e., the concept Father) with the same type of geometric representation. However, as shown on the left of Figure 1, the intersection of two $n$-balls is no longer an $n$-ball. Without the property of intersectional closure, conflicts arise when generating embeddings; for example, if the ontology contains both the axioms Parent $\sqcap$ Male $\sqsubseteq$ Father and Father $\sqsubseteq$ Male $\sqcap$ Parent, the only valid solution to finding an embedding is to make Father, Male, and Parent co-extensional; if additional axioms require Parent to contain entities that are disjoint with

![Figure 1: Example of concept intersections in 2-dimensional space.](image-url)
It is clear that, for a theory where the points that are contained within an \( n \)-box are the extension of a concept. By using the geometric interpretation of relational mappings, there is a key difference to be noted: these methods embed entities and relations in knowledge graphs from triples, while we embed concepts and relations in ontologies based on \( \mathcal{EL}^{++} \) axioms.

3 Preliminaries

In this section, we first formulate the problem we aim to solve. Then, we introduce the key terminologies in description logic \( \mathcal{EL}^{++} \) and elaborate the limitations of previous geometric embedding methods for \( \mathcal{EL}^{++} \) ontologies.

3.1 Problem Formulation

An ontology in the Description Logic \( \mathcal{EL}^{++} \) is formulated as \( \mathcal{O} = (C, R, I; ax) \) where \( C \) is a set of concept symbols, \( R \) a set of relation symbols, \( I \) a set of individual symbols, and \( ax \) a set of axioms. We aim to find an embedding \( e : \mathcal{O} \rightarrow \mathbb{R}^n \) such that the image of \( e \) is a model of \( \mathcal{O} \). Furthermore, the the embedding should allow answering queries: given a query concept description \( Q \), find all concepts \( C \) such that \( C \subseteq Q \); more specifically, we rank concepts \( C \) to find the top-\( k \) concepts that satisfy the query.

3.2 \( \mathcal{EL}^{++} \) Terminologies

In \( \mathcal{EL}^{++} \), the TBox, i.e., terminological box, contains axioms describing concept hierarchies, while the ABox, i.e., assertional box, contains axioms stating the relations between individuals (or entities) and concepts. The ABox axioms can be eliminated by replacing \( C(a) \) with \( \{a\} \subseteq C \) and replacing \( r(a, b) \) with \( \{a\} \subseteq \exists r.b \). The TBox axioms in \( \mathcal{EL}^{++} \) can be normalized into one of the seven normal forms (NFs) summarized in Table 1. The syntax and semantics of \( \mathcal{EL}^{++} \) is summarized in Table 2.
3.3 Limitations of Previous Works

Methods that construct geometric models for logical theories based on n-balls, such as ELEM [Kulmanov et al., 2019], have a crucial limitation. Representing ontology concepts as n-balls entails that they cannot represent intersections of concepts within the same formalism because intersections of n-balls are not n-balls. This does prevent embeddings based on n-balls to represent and infer equivalent concept axioms and model the second normal form (C ∩ D ⊆ E) naturally. Specifically, it leads to complications with a loss function designed to minimize the loss for the second normal form, and likely results in embeddings of lower quality as a consequence.

4 Methodology

We consider the seven types of TBox axioms in $\mathcal{EL}^{++}$ ontologies as training instances. In this section, we first detail our specially designed box-based objective functions for each type of the TBox axioms. Then we present a case study in the family domain to demonstrate the rationalness of our proposed ELBE.

4.1 First Normal Form (NF1)

We use $\beta(C)$ to represent the box embedding of concept $C$. Inspired by [Ren et al., 2020], we use two vectors to represent a box. One vector represents the center of the box and the other vector defines the offset. The center is the intersection of the diagonals. The offset is the vector that represents the size of each dimension of the box, so all the elements are non-negative values. Let $e_c: C \cup R \rightarrow \mathbb{R}^n$ be the mapping function that maps each concept to the center of its box embedding and that maps each relation to its embedding. Let $e_o: C \rightarrow \mathbb{R}^n$ be the mapping function that maps each concept to the n-dimension vector space as the offset of the box.

The loss function for the first normal form, $C \subseteq D$, aims to ensure that the box embedding of concept $C$ lies entirely within the box embedding of concept $D$. Figure 2(a) illustrates two concepts $C$ and $D$ with their two box embedding $\beta(C)$ and $\beta(D)$. The red line indicates the difference between the center vectors: $|e_c(D) - e_c(C)| = (\delta x, \delta y)$ where $\delta x$ and $\delta y$ are two non-negative real number. In Figure 2(b), we show how the red line defined by $\delta x$ and $\delta y$ is computed as $|e_c(D) - e_c(C)| + e_o(C) - e_o(D) = (\delta x, \delta y)$. As shown in Figure 2(c), when both $\delta x$, $\delta y$ are 0 or less than 0, then $\beta(D)$ will contain $\beta(C)$. When we extend to higher dimensions, if the elements of difference vector (in two dimension is $(\delta x, \delta y)$) are all less or equal to 0, then $\beta(C)$ is contained within $\beta(D)$. So the loss function of the first normal form, $C \subseteq D$, and which ensures that $\beta(C)$ is contained within $\beta(D)$ is:

$$loss_{C \subseteq D}(c, d) = ||max(zeros, |e_c(c) - e_c(d)|) + e_o(c) - e_o(d) - margin||$$ (1)

For all loss functions we use a margin vector. If all elements of margin vector are no larger than 0, then $\beta(C)$ lies properly in $\beta(D)$.

4.2 Second Normal Form (NF2)

In the embeddings space, the second norm form $C \cap D \subseteq E$ implies that the intersection of $\beta(C)$ and $\beta(D)$ is contained within $\beta(E)$. The key aim for the loss is to find the intersection of two boxes: $e_c(new) = (box_{min} + box_{max})/2$, and $e_o(new) = (box_{max} - box_{min})/2$. It will be computed using the concepts $C$ and $D$ by equation 2 and 3. We compute

$$box_{min} = max(e_c(C) - e_o(C), e_c(D) - e_o(D))$$ (2)

and

$$box_{max} = min(e_c(C) + e_o(C), e_c(D) + e_o(D))$$ (3)

from which we can obtain the center and offset of the intersection. For this new embedding representing the intersection of two concepts, we apply the same loss as for the first normal form (where concept $C$ from the first norm form is now the intersection of the concepts $C$ and $D$ in the second norm form). The loss function for the second normal form $C \cap D \subseteq E$ will be:

$$loss_{C \cap D \subseteq E}(c, d, e) = ||max(zeros, |e_c(new) - e_c(e)| + e_o(new) - e_o(e) - margin)||$$ (4)

4.3 Normal Forms with R (NF3, NF4)

The first two normal forms do not include any quantifiers or relations. Every point that lies properly within a box representing a concept is an entity that lies in the extension of the concept (see Table 2), and we apply relations as transformations on these points. We use TransE [Bordes et al., 2013]
to represent the relations between these entities. The losses in Equations 5 and 6 capture this intention; in particular, the extension of the concept \( \exists R.D \) is the transformation of all entities in the extension of \( D \) by \(-e_c(R)\).

\[
\text{loss}_{C \subseteq \exists R.D}(c, d, r) = \| \max(\text{zeros}, e_c(c)) + e_c(r) - e_c(d)\|
\]

\[
\text{loss}_{\exists R.C \subseteq D}(c, d, r) = \| \max(\text{zeros}, -e_c(c)) - e_c(r) - e_c(d)\|
\]

The loss functions in Equations 8 and 9 capture the intuition that if a concept is unsatisfiable then its embedding should have no extensions; we use a very similar loss of the normal form where \( \exists R.C \) is unsatisfiable due to our relation model based on linear transformations.

\[
\text{loss}_{C \subseteq \perp}(c) = ||e_o(c)||
\]

\[
\text{loss}_{\exists R.C \subseteq \perp}(c, r) = ||e_o(c)||
\]

We also add negatives to improve the performance of our method:

\[
\text{loss}_{C \subseteq \exists R.D}(c, d, r) = \| \max(\text{zeros}, -|e_c(c)|) + e_c(r) - e_c(d) + e_o(c) - e_o(d) + \text{margin} \|
\]

4.5 Case Study: The Family Domain

We construct a simple knowledge base to test and understand the embeddings of our model. We use the family domain in which we generate a knowledge base that contains examples for each of the normal forms (Eqn. 11–22). We chose margin \( \text{margin} = 0 \) and an embedding dimension of 2 so that we can visualize the generated embeddings in \( \mathbb{R}^2 \). As shown in Figure 3, ELBE can correctly model the relationship between each concept, especially the intersection of two concepts. In the family domain, we can infer that \( \text{Mother} \) is equivalent to the intersection of \( \text{Female} \) and \( \text{Parent} \), and \( \text{Father} \) is equivalent to the intersection of \( \text{Male} \) and \( \text{Parent} \).

\[
\text{Male} \subseteq \text{Person}
\]

\[
\text{Female} \subseteq \text{Person}
\]

\[
\text{Father} \subseteq \text{Male}
\]

\[
\text{Mother} \subseteq \text{Female}
\]

\[
\text{Father} \subseteq \text{Parent}
\]

\[
\text{Mother} \subseteq \text{Parent}
\]

\[
\text{Female} \cap \text{Male} \subseteq \perp
\]

\[
\text{Female} \cap \text{Parent} \subseteq \text{Mother}
\]

\[
\text{Male} \cap \text{Parent} \subseteq \text{Father}
\]

\[
\exists \text{hasChild}.\text{Person} \subseteq \text{Parent}
\]

\[
\text{Parent} \subseteq \exists \text{hasChild.}\top
\]
5 Experiments

In this section, we conduct extensive experiments to compare ELBE with state of the art methods by answering the following research questions:

- **RQ1**: Does the proposed box based method ELBE perform better than the state-of-the-art methods?
- **RQ2**: How does satisfying intersectional closure contribute to learning \( E \mathcal{L}^+ \) embeddings?

5.1 Experimental settings

**Datasets.** Following the well-established previous works [Kulmanov et al., 2019], we use two real-world benchmark datasets to evaluate ELBE: the datasets are used to predict protein–protein interactions (PPIs) in yeast and humans. Each protein is associated with its biological functions as expressed using the Gene Ontology (GO) [Ashburner et al., 2000], and interactions are predicted based on the biological hypothesis that proteins that are functionally similar are more likely to interact. We use the OWL representation of the datasets where proteins are instances, and if protein \( P \) is associated with the function \( F \), we add the axiom \( \{ P \} \sqsubseteq \exists \text{hasFunction},F \) (based on the ABox axiom \( \exists \text{hasFunction},F(P) \)). We use 80% of the total interacted protein pairs for model training, 10% and 10% for validation and testing, respectively.

In addition, we generate a synthetic dataset to evaluate the performance of ELBE on the inference of equivalence concept axioms. The details of this task are in Section 5.3. For generating the dataset, we choose the GO as the basic dataset, then randomly choose 2,131 axioms of NF2 \((C \sqsubseteq D) \sqsubseteq E\). Then, for each NF2 axiom we chose, we add the axioms \( C \sqsubseteq E \) and \( D \sqsubseteq E \) axioms to the dataset. The two NF1 axioms and one NF2 axiom form a triple that we use for the entailment of equivalence concepts. We randomly choose 1,000 of these triples for evaluation and use the rest for training the embeddings.

**Baselines.** We compare ELBE with TransE [Bordes et al., 2013], Resnik’s similarity [Resnik, 1995], Lin’s similarity [Harispe et al., 2015], EmEL++ [Mondala et al., 2021], ELEm [Kulmanov et al., 2019]. For TransE, we use two representations, a native RDF-based rendering of the OWL knowledge base, and a “plain” representation based on OWL2Vec* [Chen et al., 2021] transformation rules, to generate knowledge graph embeddings and use them for link prediction. For Resnik’s similarity and Lin’s similarity, we use the best-match average strategy for combining pairwise class similarities, then compute the similarity between each protein. For EmEL++ and ELEm, we predict whether axioms of the type \( P_1 \sqsubseteq \exists \text{interacts},P_2 \) hold.

**Implementation Details.** We implement ELBE using the Python library PyTorch\(^1\) and conduct all the experiments on a Linux server with GPUs (Nvidia RTX 2080Ti) and Intel Xeon CPU. In the training phase, the initial learning rate of the Adam [Kingma and Ba, 2014] optimizer is tuned by grid searching within \( \{1e^{-2}, 5e^{-3}, 1e^{-3}, 5e^{-4}\} \) for both tasks. We perform an extensive search for optimal parameters, testing embedding sizes for \( \{25, 50, 100, 200, 400\} \) and margin vectors for \( \{-0.01, -0.05, -0.01, 0, 0.01, 0.05, 0.1\} \). The optimal set of key hyper-parameters for ELBE is \( \text{embedding size} = 50, \text{margin} = -0.05 \).

For the PPI task, we evaluate the performance based on hit rate at ranks 10 (H@10) and 100 (H@100), mean rank (MR) and area under the ROC curve (AUC) and report both raw and filtered results (e.g., MR(F) indicates mean rank of the filtered result). For entailment of equivalent concepts, we evaluate the performance based on hit rate at ranks 1, 3, and 10, and the mean rank. You can see our code at github\(^2\).

5.2 Protein–Protein Interactions (RQ1)

We use the similarity-based function in Eqn 23 for predicting PPIs.

\[
sim(P_1, \text{interact}, P_2) = -||\max(\text{zeros}, |e_c(P_1)|) + e_c(\text{interact}) - e_c(P_2)| - e_o(P_1) - e_o(P_2)||
\]

(23)

For a query \( P_1 \sqsubseteq \exists \text{interacts},P_2 \), we predict interactions of \( P_2 \) to all proteins from our training set and identify the rank of \( P_1 \).

We compare the overall performance of ELBE with that of baselines to answer RQ1. The results are shown in Table 3 for the yeast PPI dataset and in Table 4 for the human PPI dataset. The results shows that ELBE consistently outperforms other baselines.

5.3 Entailment of Equivalence Concepts (RQ2)

ELBE outperforms other methods in our experiments, and we hypothesize this is due to the improved representation of concept intersections. We perform a more thorough analysis of ELBE’s ability to represent and infer intersections. In the knowledge base based on GO, if there are three axioms of the form \( E \sqsubseteq C, E \sqsubseteq D \), \( E \sqcap D \sqsubseteq E \), then we can infer (deductively) that \( C \sqsubseteq D \sqsubseteq E \). We perform an experiment to test whether ELBE is able to make these inferences within the embedding space.

To the best of our knowledge, the current methods for \( \mathcal{E} \mathcal{L}^+ \) embeddings are all based on geometric models based on \( n \)-balls; we used ELEm [Kulmanov et al., 2019] as representative.

To do the entailment of equivalence concepts task, we predict which concept equals the intersection of two other concepts. Intuitively, we should calculate the intersection of concepts first and then compare the intersection to the embedding of each concept, and choose the closest one. However, ELEm only approximate the intersection and do not actually represent it; therefore, we use the center of the smallest \( n \)-ball containing the intersection as representation of the concept and choose the concept that has the closest center of its \( n \)-ball embedding. The similarity-based function for ELEm is in equation 26.

\[
h = \frac{r_q(C)^2 - r_q(D)^2 + ||f_q(D) - f_q(C)||^2}{2||f_q(D) - f_q(C)||}
\]

(24)

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\(^1\)https://pytorch.org/

\(^2\)https://github.com/bio-ontology-research-group/EL2Box_embedding
### Table 3: Prediction performance for yeast protein–protein interactions.

| Method   | H@10(R) | H@10(F) | H@100(R) | H@100(F) | MR(R) | MR(F) | AUC(R) | AUC(F) |
|----------|---------|---------|----------|----------|-------|-------|--------|--------|
| TransE(R) | 0.03    | 0.05    | 0.22     | 0.27     | 855   | 809   | 0.84   | 0.85   |
| TransE(P) | 0.06    | 0.13    | 0.41     | 0.54     | 378   | 330   | 0.93   | 0.94   |
| SimResnik | 0.08    | 0.18    | 0.38     | 0.49     | 713   | 663   | 0.87   | 0.88   |
| SimLin    | 0.08    | 0.17    | 0.34     | 0.45     | 807   | 756   | 0.85   | 0.86   |
| EmEL++    | 0.07    | 0.17    | 0.48     | 0.65     | 336   | 291   | 0.94   | 0.95   |
| ELEm      | 0.10    | 0.23    | 0.50     | 0.75     | 247   | 187   | 0.96   | 0.97   |
| **ELBE**  | **0.11**| **0.26**| **0.57** | **0.77** | **201**| **154**| **0.96**| **0.97**|

### Table 4: Prediction performance for human protein–protein interactions.

| Method   | H@10(R) | H@10(F) | H@100(R) | H@100(F) | MR(R) | MR(F) | AUC(R) | AUC(F) |
|----------|---------|---------|----------|----------|-------|-------|--------|--------|
| TransE(R) | 0.02    | 0.03    | 0.12     | 0.16     | 2262  | 2189  | 0.85   | 0.85   |
| TransE(P) | 0.05    | 0.11    | 0.32     | 0.44     | 809   | 737   | 0.95   | 0.95   |
| SimResnik | 0.05    | 0.10    | 0.23     | 0.28     | 2549  | 2476  | 0.83   | 0.83   |
| SimLin    | 0.04    | 0.08    | 0.19     | 0.22     | 2818  | 2743  | 0.81   | 0.82   |
| EmEL++    | 0.04    | 0.13    | 0.38     | 0.56     | 772   | 700   | 0.95   | 0.95   |
| ELEm      | 0.09    | 0.22    | 0.43     | 0.70     | 658   | 572   | 0.96   | 0.96   |
| **ELBE**  | **0.09**| **0.22**| **0.49** | **0.72** | **434**| **362**| **0.97**| **0.98**|

### Table 5: Performance for entailment of equivalence concepts tasks.

| Method | H@1 | H@3 | H@10 | MR  |
|--------|-----|-----|------|-----|
| ELEm   | 0.710 | 0.896 | 0.969 | 3.561 |
| ELBE   | 0.871 | 0.974 | 0.985 | 3.470 |

In this similarity function, $r_{eta}$ and $f_{eta}$ are the radius and center of the $n$-ball of the ELEm. The similarity-based function for ELBE is in equation 27:

$$sim_{ball}(C, D, E) = |f_{eta}(C) + k(f_{eta}(D) - f_{eta}(C)) - f_{eta}(E)|$$

In the test triples, ELBE can predict over 87% of the equivalence axioms correctly, while ELEm can predict only 71%. In other word, by satisfying the intersectional closure, ELBE can perform entailment of equivalence accurately. Solving the intersectional closure problem is a crucial step towards establishing a correspondence between vector space embeddings and models of axiomatic theories.

### 7 Future Work

One limitation of ELBE is the use of TransE as model for relations. TransE can only deal with one-to-one relations, while one-to-many and many-to-many relations are important for accurately embedding ontologies. Furthermore, TransE is a linear transformation model; consequently, some of our loss functions (in particular $loss_{3R,C \subseteq \perp}$) are insufficient to capture the $\mathcal{EL}^{++}$semantics. In future work, we will explore more expressive relation models for $\mathcal{EL}^{++}$embedding.
to solve these limitations.
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