

ACHIEVING HYPERBOLIC-LIKE EXPRESSIVENESS WITH ARBITRARY EUCLIDEAN REGIONS: A NEW APPROACH TO HIERARCHICAL EMBEDDINGS

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ABSTRACT

Hierarchical data is common in many domains like life sciences and e-commerce, and its embeddings often play a critical role. While hyperbolic embeddings offer a theoretically grounded approach to representing hierarchies in low-dimensional spaces, current methods often rely on specific geometric constructs as embedding candidates. This reliance limits their generalizability and makes it difficult to integrate with techniques that model semantic relationships beyond pure hierarchies, such as ontology embeddings. In this paper, we present RegD, a flexible Euclidean framework that supports the use of arbitrary geometric regions—such as boxes and balls—as embedding representations. Although RegD operates entirely in Euclidean space, we formally prove that it achieves hyperbolic-like expressiveness by incorporating a depth-based dissimilarity between regions, enabling it to emulate key properties of hyperbolic geometry, including exponential growth. Our empirical evaluation on diverse real-world datasets shows consistent performance gains over state-of-the-art methods and demonstrates RegD’s potential for broader applications such as the ontology embedding task that goes beyond hierarchy.

1 INTRODUCTION

Embedding discrete data into low-dimensional vector spaces has become a cornerstone of modern machine learning. In Natural Language Processing (NLP), seminal works such as word2vec Mikolov et al. (2013) and GloVe Pennington et al. (2014) represent words as vectors to capture intricate linguistic relationships. Similarly, knowledge graph embedding methods Bordes et al. (2013); Sun et al. (2019); Balazevic et al. (2019) encode entities and relations as vectors with their semantics concerned to facilitate reasoning and prediction.

Our work focuses on embedding hierarchical data into low-dimensional spaces. Such data represents partial orders over sets of elements, denoted as $u \prec v$, where u is a parent of v . These partial orders naturally manifest as trees or directed acyclic graphs (DAGs). The ability to effectively embed such hierarchical structures enables crucial operations like inferring sub- or superclasses of concepts and classifying nodes within graphs. These capabilities are essential for various tasks in knowledge management and discovery, particularly towards knowledge bases Shi et al. (2024); Abboud et al. (2020), ontologies He et al. (2024a); Chen et al. (2024) and taxonomies Shen & Han (2022).

Current methods for embedding hierarchical data can be broadly categorized into two paradigms: *region-based* and *hyperbolic* approaches. The region-based approach usually represents entities as geometric regions in the Euclidean space, capturing hierarchical relationships through intuitive region-inclusion. However, these methods often experience degraded performance in low-dimensional settings due to the crowding effect inherent in Euclidean spaces.

In contrast, the hyperbolic approach takes advantage of the unique geometric properties of hyperbolic spaces—specifically their exponential growth in distance and volume—enabling more effective embeddings of tree-structured data in low dimensions. However, as shown in Table 1, existing hyperbolic methods often rely on specialized constructed objects as embedding candidates Ganea et al. (2018b); Yu et al. (2024), limiting their generalizability to data that encodes richer semantics beyond hierarchy. For example, EntailmentCones Ganea et al. (2018b) and ShadowCones Yu et al. (2024) are not closed under intersection and thus cannot handle conjunction.

Method	Embeddings of a node u	Energy/score function for $u \prec v$
Poincaré Nickel & Kiela (2017)	Points $\mathbf{u} \in \mathbb{H}^d$	$(1 + \alpha(\ \mathbf{u}\ - \ \mathbf{v}\))d_k(\mathbf{u}, \mathbf{v})$
EntailmentCones Ganea et al. (2018b)	Cones with apex $\mathbf{u} \in \mathbb{H}^d$ and angle $\theta_{\mathbf{u}} = \arcsin(\frac{(1-\ \mathbf{u}\ ^2)}{\ \mathbf{u}\ })$	Angle-based function
ShadowCones Yu et al. (2024)	Cones with apex $\mathbf{u} \in \mathbb{H}^d$ and angle $\theta_{\mathbf{u}} = \arctan \sinh(\sqrt{kr})$	$d_{\mathbb{H}}(\mathbf{u}, \mathbf{v})$ or specific boundary distance
RegD (ours)	arbitrary regions in \mathbb{R}^d (e.g., balls, boxes)	$d_{\text{bd}}(\text{reg}_u, \text{reg}_v) + \lambda \cdot d_{\text{dep}}(\text{reg}_u, \text{reg}_v)$

Table 1: Comparison with hyperbolic methods in \mathbb{H}^d (curvature $-k$, distance d_k). α , r and λ are predefined hyperparameters. Only the umbral half-space model of ShadowCones is shown, with boundary distance defined in Eq. 6.

In this paper, we propose a flexible framework named RegD for modeling hierarchical data by embedding arbitrary regions in Euclidean spaces. Our framework relies on two novel dissimilarity metrics, *depth dissimilarity* d_{dep} and *boundary dissimilarity* d_{bd} , which combine the strengths of both region-based approaches in Euclidean spaces and hyperbolic methods. **The depth dissimilarity** (cf. Section 3.1) enables our model to achieve embedding expressiveness comparable to that of hyperbolic spaces by incorporating the “size” of the regions under consideration (cf. Theorem 1 and Propositions 1 and 3). **The boundary dissimilarity** (cf. Section 3.2) improves the representation of set-inclusion relationships among regions in Euclidean spaces. This allows for better identification of shallower and deeper descendants, thereby capturing hierarchical structures more effectively than traditional region-based approaches (cf. Proposition 2). Note that these dissimilarities may be negative or fail to satisfy the triangle inequality, and thus are generally not strict metric distances.

Notably, RegD can be applied to arbitrary regions, including common geometric representations such as balls and boxes. This generality enables broad applicability across diverse geometric embeddings for various tasks, extending beyond hierarchy alone data to ontologies that include hierarchies and more complex relationships in Description Logic Baader et al. (2017) (cf. Sections 4.2 and 4.3). Our main contributions are summarized as follows:

- We present a versatile framework that is able to embed hierarchical data as arbitrary regions in Euclidean space.
- We offer a rigorous theoretical analysis demonstrating that our framework retains the core embedding benefits of hyperbolic methods.
- Experiments on diverse real-world datasets demonstrate that our framework consistently outperforms existing approaches on embedding hierarchies and ontologies for reasoning and prediction.

For brevity, all proofs of theorems and properties are provided in Appendix A.

2 PRELIMINARIES AND RELATED WORKS

Manifold and Hyperbolic Space A d -dimensional *manifold* Lee (2013), denoted \mathcal{M} , is a hypersurface embedded in an n -dimensional Euclidean space, \mathbb{R}^n , where $n \geq d$, and locally resembles \mathbb{R}^d . A *Riemannian manifold* \mathcal{M} is a manifold equipped with a Riemannian metric, enabling the definition of a distance function $d_{\mathcal{M}}(\mathbf{x}, \mathbf{y})$ for $\mathbf{x}, \mathbf{y} \in \mathcal{M}$. *Hyperbolic space*, denoted \mathbb{H}^n , is a Riemannian manifold with a constant negative curvature of $-k$, where $k > 0$ Lee (2006). It can be represented using various isometric models, such as the Poincaré ball model (see Appendix C) or Poincaré half-space model, where the points are defined by the half-space: $U^n = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{x}_n > 0\}$, and the hyperbolic distance between $\mathbf{x}, \mathbf{y} \in U^n$ is given by $d_k(\mathbf{x}, \mathbf{y}) = \frac{1}{\sqrt{k}} \operatorname{arcosh} \left(1 + \frac{\|\mathbf{x} - \mathbf{y}\|_2^2}{2\mathbf{x}_n \mathbf{y}_n} \right)$.

Region-based Methods Region-based methods embed the nodes of a directed acyclic graph (DAG) into regions on Euclidean space or Riemannian manifolds, such as boxes Boratko et al. (2021); Zhang et al. (2022), balls Suzuki et al. (2019), and cones Vendrov et al. (2016), capturing hierarchical relationships through set-inclusion between these regions. Training is typically conducted using an inclusion loss, which is often defined in terms of the distance or volume of the regions Vendrov et al.

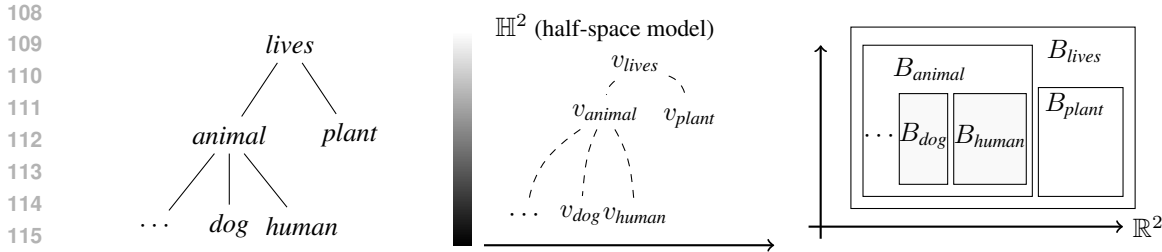


Figure 1: Demonstration of a taxonomy (left), its embeddings in the hyperbolic space (middle) and in the Euclidean space as boxes (right).

(2016). However, such loss functions may involve non-smooth operations, like maximization, which have been addressed through probabilistic Vilnis et al. (2018); Dasgupta et al. (2020) or smooth Boratko et al. (2021) approximations to improve performance. However, most of these methods suffer from the crowding effect in Euclidean space, which limits their expressiveness compared to our method and hyperbolic-based approaches.

Hyperbolic Methods Hyperbolic space embeddings Nickel & Kiela (2017); Sonthalia & Gilbert (2020); Sala et al. (2018) have been introduced to model hierarchical structures by leveraging favorable properties of hyperbolic space, such as its exponential growth. However, these methods primarily rely on pointwise distances to encode hierarchies, which is less intuitive for representing transitivity properties. In contrast, *EntailmentCones* Ganea et al. (2018b), and *ShadowCones* propose using regions in hyperbolic space that capture hierarchies through set inclusion, which can be regarded as region-based methods in hyperbolic spaces. Specifically, *EntailmentCones* introduces closed-form hyperbolic cones, defined by their apex coordinates, while *ShadowCones* use different cones are inspired by the physical interplay of light and shadow. However, as shown in Table 1, these regions all take specific forms, limiting their generalizability to other tasks or methods.

3 METHOD

3.1 DEPTH DISSIMILARITY: A SIMILARITY MEASURE INCORPORATING DEPTH

Unlike the Euclidean space, which is constrained by crowding effects that limit its embedding capacity, the hyperbolic space leverages exponential growth in distance and volume to offer superior embedding capabilities. This property makes the hyperbolic space particularly effective for representing tree-structured data in low-dimensional spaces. Notably, two key distinctions arise between region-based embeddings in the Euclidean space and hyperbolic embeddings:

1. *The hyperbolic space better discriminates different hierarchical layers than the Euclidean space.*

Consider the taxonomy illustrated in Figure 1 (left). Intuitively, since *human* is a subcategory of *animal*, the semantic difference between *human* and *plant* should be greater than that between *animal* and *plant*. The hyperbolic space effectively captures this hierarchical relationship by permitting $d(v_{human}, v_{plant}) > d(v_{animal}, v_{plant}) + \Delta$, where Δ is an arbitrary gap. This arises from the property that the distance metric diverges to infinity near the boundary, as illustrated by the shadow dense of the bar on the left-hand side of \mathbb{H}^2 in Figure 1 (middle). In contrast, region-based embeddings on Euclidean space may violate this hierarchical constraint, potentially placing the box B_{human} close to B_{plant} , resulting in a distance (e.g., the Euclidean distance between box centers) similar to or even smaller than that between B_{animal} and B_{plant} .

2. *The hyperbolic space enables the distinct representation of an arbitrary number of child nodes.*

As demonstrated in Figure 1, the box embeddings in the Euclidean space face inherent limitations when representing multiple children of a node, such as *animal*. As the number of children increases, their corresponding boxes must cluster within B_{animal} , leading to crowding. In contrast, the hyperbolic space can accommodate an arbitrary number of children while maintaining distinct separations between them. This capability arises from the exponential growth of distance near the boundary of the hyperbolic space, which allows unlimited child nodes to be positioned distinctly

by placing them progressively closer to the boundary while preserving meaningful distances between them.

In the following sections, we introduce the notion of *depth dissimilarity* for regions in Euclidean space, which explicitly accounts for their “size.” We show that this measure retains advantages analogous to those of hyperbolic spaces (Theorem 1), while offering a simpler structure that facilitates implementation (e.g., avoiding specialized techniques such as double-precision tensors and Riemannian-specific optimizers Bécigneul & Ganea (2019)) and enabling potential extensions (e.g., integration with ontology embeddings; see Section 4.2). Moreover, we establish that depth dissimilarity encompasses hyperbolic distance as a special case (Proposition 1), while providing greater flexibility by preserving key properties of hyperbolic geometry through simple polynomial functions (Proposition 2).

Construction The depth dissimilarity serves as a similarity measure that quantifies the relationship between objects considering their hierarchical depth. As we use set-inclusion relations to model the hierarchy, this hierarchical depth can be represented through the size of the regions, such as their volumes or diameters. Formally, the depth dissimilarity is defined as follows, where the size of the regions is represented by a function $f(\text{reg})$:

Definition 1 (Depth Dissimilarity). *Let \mathcal{R} be a collection of parameterized regions¹ in the n -dimensional Euclidean space \mathbb{R}^n , i.e., each region $\text{reg} \in \mathcal{R}$ is characterized by an m -dim parameter $P(\text{reg}) \in \mathbb{R}^m$. The depth dissimilarity between two regions $\text{reg}_1, \text{reg}_2 \in \mathcal{R}$, is defined as:*

$$d_{\text{dep}}(\text{reg}_1, \text{reg}_2) = g\left(\frac{\|P(\text{reg}_1) - P(\text{reg}_2)\|_p^p}{f(\text{reg}_1)f(\text{reg}_2)}\right) \quad (1)$$

where $\|\cdot\|_p$ is the p -norm (i.e., $\|\mathbf{x}\|_p = (\sum_i x_i^p)^{1/p}$), and:

- $g : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}_{\geq 0}$ is an increasing function such that $g(x) = 0$ if and only if $x = 0$,
- $f : \mathcal{R} \rightarrow \mathbb{R}_{> 0}$ is a function that measures the size of regions. It satisfies: $\lim_{\text{reg} \rightarrow \emptyset} f(\text{reg}) = 0^2$.

We require f and g to have non-negative values to ensure the depth dissimilarity is non-negative. Additionally, we stipulate that $\lim_{\text{reg} \rightarrow \emptyset} f(\text{reg}) = 0$ to guarantee that as a region shrinks to an empty set, the dissimilarity between this object and others can approach infinity. This setting emulates the beneficial properties of the hyperbolic space, where the dissimilarity between two points can grow rapidly as they approach the boundary of the space (i.e., $x_n = 0$ in the Poincaré half-space model). In our context, the boundary of the space \mathcal{R} of a collection of (parametrized) regions in the Euclidean space is the empty set. By selecting an appropriate function f , we can control the rate at which the dissimilarity between two objects increases as they approach this boundary.

For the remainder of this paper, we restrict our theoretical analysis and implementations to boxes and balls as representative region types for clarity and tractability. It is important to note, however, that the theoretical results established herein naturally extend to other parameterized region representations, with analogous proof techniques applicable. For details, please refer to Appendix A.5.

Example 1. Let $\text{ball}(\mathbf{c}, r) = \{\mathbf{x} \mid \|\mathbf{x} - \mathbf{c}\| \leq r\}$ be a ball defined by a center $\mathbf{c} \in \mathbb{R}^n$ and a radius $r > 0$. By setting $g(x) = x$ and $f(\text{ball}) = r$, we obtain a depth dissimilarity of the form:

$$d_{\text{dep}}(\text{ball}_1(\mathbf{c}_1, r_1), \text{ball}_2(\mathbf{c}_2, r_2)) = \frac{\|\mathbf{c}_1 - \mathbf{c}_2\|_p^p + |r_1 - r_2|^p}{r_1 \cdot r_2}. \quad (2)$$

Example 2. Let $\text{box}(\mathbf{c}, \mathbf{o}) = \{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{c} - \mathbf{o} \leq \mathbf{x} \leq \mathbf{c} + \mathbf{o}\}$ be a box defined by a center $\mathbf{c} \in \mathbb{R}^n$ and an offset $\mathbf{o} \in \mathbb{R}_{> 0}^n$. By setting $g(x) = x$ and $f(\text{box}) = \|\mathbf{o}\|$, we obtain a depth dissimilarity:

$$d_{\text{dep}}(\text{box}_1(\mathbf{c}_1, \mathbf{o}_1), \text{box}_2(\mathbf{c}_2, \mathbf{o}_2)) = \frac{\|\mathbf{c}_1 - \mathbf{c}_2\|_p^p + \|\mathbf{o}_1 - \mathbf{o}_2\|_p^p}{\|\mathbf{o}_1\| \cdot \|\mathbf{o}_2\|}. \quad (3)$$

The following result highlights that the depth dissimilarity exhibits properties analogous to those of the hyperbolic distance discussed earlier in this section. Specifically, the depth dissimilarity **(1)**

¹See Appendix A.5 for a formal definition. Examples as boxes and balls are shown in Example 1, 2.

² $\text{reg} \rightarrow \emptyset$ indicates that the region reg shrinks to the empty set (e.g., its volume or diameter tends to zero).

effectively distinguishes concepts across different layers of the hierarchy with an arbitrary separation gap, denoted by Δ in item 1 of the following Theorem 1, and (2) distinctly represents an arbitrary number n of children within a single parent by a dissimilarity greater than M , as demonstrated in item 2 of the theorem.

Theorem 1. Consider the region space \mathcal{B}^n consisting of balls in \mathbb{R}^n , with the depth dissimilarity defined in Example 1. The following properties hold:

1. For any ball₁, ball₂ $\in \mathcal{B}^n$ and any $\Delta > 0$, there exists a positive constant r_0 such that for any ball(\mathbf{c}' , r') \subseteq ball₂, if $r' \leq r_0$, then $d_{dep}(\text{ball}_1, \text{ball}(\mathbf{c}', r')) > d_{dep}(\text{ball}_1, \text{ball}_2) + \Delta$.
2. For any ball $\in \mathcal{B}^n$, any integer n and any $M > 0$, there exist subsets ball₁, ..., ball_n \subseteq ball such that for any distinct $i, j \in \{1, \dots, n\}$, we have $d_{dep}(\text{ball}_i, \text{ball}_j) > M$.

The same conclusions hold for boxes, where $r_0 \in \mathbb{R}_{>0}$ is replaced with $\mathbf{o}_0 \in (\mathbb{R}_{>0})^n$, and the condition $r' \leq r_0$ is replaced by $\mathbf{o}' \leq \mathbf{o}_0$ element-wise.

Comparison with the Hyperbolic Distance The following theorem shows that our depth dissimilarity encompasses hyperbolic distance as a special case, obtained with specific choices of functions f, g in Definition 1.

Proposition 1. Let \mathbb{H}^{n+1} be the hyperbolic space with curvature -1 . Assume the ball space \mathcal{B}^n is parameterized as in Example 1, and equipped with the depth dissimilarity defined in Equation (1). Then the map $F: \mathcal{B}^n \rightarrow \mathbb{H}^{n+1}$ defined by $F(\text{ball}(\mathbf{c}, r)) = [\mathbf{c} : r]$ is a bijective isometry when $p = 2$, $g(x) = \text{arcosh}(x + 1)$, and $f(\text{ball}(\mathbf{c}, r)) = \sqrt{2}r$.

Moreover, the following result demonstrates that even with a simple linear function $g(\cdot)$, our depth dissimilarity retains the ability to capture the hyperbolic structure. Specifically, there exists a map from the region space to the hyperbolic space that preserves the order of hyperbolic distances for all pairs of points, as stated below.

Proposition 2. Following Proposition 1, let the depth dissimilarity d_{dep} be redefined by replacing g to $g(x) = k \cdot x$ ($k > 0$). Then the map F retains the following monotonicity property: for any points $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4 \in \mathbb{H}^n$, $d_{\mathbb{H}^n}(\mathbf{x}_1, \mathbf{x}_2) < d_{\mathbb{H}^n}(\mathbf{x}_3, \mathbf{x}_4)$ if and only if

$$d_{dep}(F^{-1}(\mathbf{x}_1), F^{-1}(\mathbf{x}_2)) < d_{dep}(F^{-1}(\mathbf{x}_3), F^{-1}(\mathbf{x}_4)).$$

It is important to recognize that evaluation metrics such as F1 scores and Hits@k rely solely on the ranking induced by the scoring function. As a result, only the relative order of the scores matters, while their absolute values are less important. Therefore, preserving the same ranking as that produced by hyperbolic distances is sufficient to attain comparable performance. Consequently, the depth-based dissimilarity defined in Equations 2 and 3, with the function $g(x) = x$, are well-suited for our implementation, as justified by Proposition 3.

3.2 BOUNDARY DISSIMILARITY: A NON-SYMMETRIC MEASURE OF INCLUSION

Although the depth dissimilarity d_{dep} introduced above has been shown to have great power for embedding hierarchical data, it is a symmetric metric and therefore inadequate for fully capturing the inherently non-symmetric hierarchical relationships between objects. To address this limitation, we introduce the boundary dissimilarity, specifically designed to reflect the partial order of regions defined by set inclusion.

Our boundary dissimilarity generalizes the signed-distance-to-boundary in ShadowCone (Theorem 4.2, Yu et al. (2024)) by extending its applicability from specialized hyperbolic cone geometries to arbitrary Euclidean regions. This generalization is formally defined in Definition 2. As a result, our boundary dissimilarity can be computed in a much simpler form (Example 3) compared to the formulation used in ShadowCone (Equation 6).

Construction The boundary dissimilarity is defined to measure the minimal cost associated with transforming the spatial relationship between two regions reg_1 and reg_2 . Specifically, it quantifies the cost of moving reg_2 out of reg_1 when $reg_2 \subseteq reg_1$, or moving reg_2 into reg_1 otherwise (when $reg_2 \not\subseteq reg_1$). This cost can be defined for arbitrary geometric objects based on either distance or

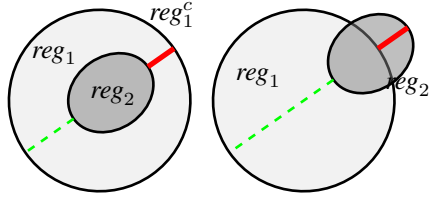


Figure 2: Illustration of $d_{bd}(reg_1, reg_2)$ (red) for $reg_2 \subseteq reg_1$ (left) or $reg_2 \not\subseteq reg_1$ (right). Green lines shows the inverse: $d_{bd}(reg_2, reg_1)$.

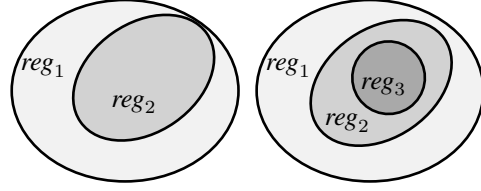


Figure 3: Illustration of internally tangent of item 1 (left) and item 2 (right) in Proposition 3.

volume within Euclidean or other spaces. Below, we introduce a boundary dissimilarity based on the Euclidean distance for two regions $reg_1, reg_2 \subseteq \mathbb{R}^n$, which consists of two cases:

1. *Containment* ($reg_2 \subseteq reg_1$): As illustrated in the left of Figure 2, when reg_2 is fully contained within reg_1 , the boundary dissimilarity is defined by the minimum Euclidean distance between the complementary region reg_1^c and the points in reg_2 (i.e., length of the red line). This distance quantifies the minimum translation cost required to move at least a part of reg_2 out of reg_1 .
2. *Non-Containment* ($reg_2 \not\subseteq reg_1$): As shown in the right of Figure 2, when reg_2 is not fully contained within reg_1 , the boundary dissimilarity is defined as the maximum Euclidean distance from the points in $reg_2 \setminus reg_1$ to reg_1 (i.e., length of the red line). This distance quantifies the minimum translation cost for moving reg_2 into reg_1 .

Let $d(reg, \mathbf{x}) := \min\{\|\mathbf{x} - \mathbf{y}\|_2 \mid \mathbf{y} \in reg\}$ be the distance of a points \mathbf{x} to a region reg defined by the minimal distance from \mathbf{x} to $\mathbf{y} \in reg$. The formal definition of the boundary dissimilarity is as follows:

Definition 2 (Boundary Dissimilarity). *Given a region space \mathcal{R} , we define the boundary dissimilarity over $reg_1, reg_2 \in \mathcal{R}$ by:*

$$d_{bd}(reg_1, reg_2) = \begin{cases} - \min_{\mathbf{x}_2 \in reg_2} \{d(reg_1^c, \mathbf{x}_2)\} & \text{if } reg_2 \subseteq reg_1 \\ \max_{\mathbf{x}_2 \in reg_2 \setminus reg_1} \{d(reg_1, \mathbf{x}_2)\} & \text{else.} \end{cases} \quad (4)$$

Note that a negative sign is added to $d_{bd}(reg_1, reg_2)$ in the containment case ($reg_2 \subseteq reg_1$) to clearly distinguish it from other cases. Moreover, the boundary dissimilarity is inherently asymmetric, that is, $d_{bd}(reg_1, reg_2) \neq d_{bd}(reg_2, reg_1)$ in general. For example, as illustrated in Figure 2, the boundary dissimilarity in the reverse order, $d_{bd}(reg_2, reg_1)$, corresponds to the length of the green dashed line, which differs from the red line representing $d_{bd}(reg_1, reg_2)$.

Moreover, for widely used geometric objects such as balls and boxes, the boundary dissimilarity can be computed efficiently using simple arithmetic operations.

Example 3. *If $reg_1 = ball(\mathbf{c}_1, r_1)$ and $reg_2 = ball(\mathbf{c}_2, r_2)$, the boundary dissimilarity have the form (here the two cases can be unified into a single formula):*

$$d_{bd}(reg_1, reg_2) = \|\mathbf{c}_1 - \mathbf{c}_2\|_2 + r_2 - r_1$$

For the case of boxes, where $reg_1 = box(\mathbf{c}_1, \mathbf{o}_1)$ and $reg_2 = box(\mathbf{c}_2, \mathbf{o}_2)$, the boundary dissimilarity have the form:

$$d_{bd}(reg_1, reg_2) = \begin{cases} \max(|\mathbf{c}_1 - \mathbf{c}_2| + \mathbf{o}_2 - \mathbf{o}_1) & \text{if } reg_2 \subseteq reg_1, \\ \|\max\{|\mathbf{c}_1 - \mathbf{c}_2| + \mathbf{o}_2 - \mathbf{o}_1, \mathbf{0}\}\|_2 & \text{else.} \end{cases}$$

Here, $\max(\cdot)$ in the first line denotes the maximal value along all dimensions, while $\max\{\cdot, \cdot\}$ in the second line applies element-wise to the two vectors or values.

The following proposition demonstrates that our definition of the boundary dissimilarity effectively captures the inclusion relationship between two regions in two key aspects, as illustrated in Figure 3: (i) it identifies whether one region is (exactly) contained within another, and (ii) it enhances

discrimination in inclusion chains, as smaller regions tend to have larger boundary dissimilarities. This property is useful for distinguishing shallow children from deeper ones. It is worth noting that the proposition below applies to any regions, not only boxes or balls.

Proposition 3. *For the boundary dissimilarity d_{bd} in Definition 2, the following properties hold:*

1. $d_{bd}(reg_1, reg_2) \leq 0$ if and only if $reg_1 \subseteq reg_2$. Moreover, $d_{bd}(reg_1, reg_2) = 0$ if and only if reg_1 is internally tangent to reg_2 . That is, $reg_1 \subseteq reg_2$, and their boundaries intersect at some point.
2. If $reg_3 \subseteq reg_2 \subseteq reg_1$, then $d_{bd}(reg_1, reg_3) \leq d_{bd}(reg_1, reg_2)$.

Specific Constructions for Boxes or Balls For specific geometric regions like balls and boxes, we can create specialized distance functions to measure the set-inclusion relationship based on their intrinsic geometric properties or established methods. Our framework accommodates these specialized metrics by allowing them to replace the general boundary dissimilarity function.

1. *Volume-based dissimilarity for boxes:* Since the volume of a box can be computed as the product of its offsets along different dimensions, we can define a partial distance based on volume:

$$d_{vol}(reg_1, reg_2) = -\ln \left(\frac{\text{vol}(reg_1 \cap reg_2)}{\text{vol}(reg_2)} \right). \quad (5)$$

2. *Hyperbolic dissimilarity for balls:* Yu et al. (2024) introduced a series of circular cones in hyperbolic space and defined a boundary dissimilarity based on the hyperbolic distance between the apex of these cones. By utilizing the natural mapping from balls to circular cones, we can derive a new boundary dissimilarity for balls as follows (see Appendix B for more details):

$$d_{bd}^{\text{cone}}(reg_1, reg_2) = \text{arcsinh} \left(\frac{\|\mathbf{c}_1 - \mathbf{c}_2\|_2 - r_1}{r_2} \right) + \text{arcsinh}(1) \quad (6)$$

3.3 TRAINING

For a given pair (u, v) , we define their energy as a weighted sum with weight λ that balances the contributions of the hyperbolic-like depth dissimilarity:

$$E(u, v) = d_{bd}(reg_u, reg_v) + \lambda \cdot d_{dep}(reg_u, reg_v), \quad (7)$$

We say that u is considered a parent of v (i.e., $u \prec v$) if $E(u, v) \leq t$, where t is a threshold that achieved the best performance on the evaluation set.

For model training, we use d_{dep} from Equation 2 or 3 with the contrastive loss from Yu et al. (2024):

$$\mathcal{L}(\gamma_1, \gamma_2) = \sum_{(u,v) \in P} \left(\max\{E(u, v), \gamma_1\} + \log \left(\sum_{(u,v') \in N} e^{\max\{\gamma_2 - d_{bd}(reg_u, reg_{v'}), 0\}} \right) \right), \quad (8)$$

where P and N denote positive and negative sample pairs, respectively. For **positive pairs** $(u, v) \in P$, the loss based on $E(u, v)$ promotes both the containment of reg_v within reg_u (via the d_{bd} term) and their geometric similarity (via the d_{dep} term), whose contributions are controlled by the weight λ and the threshold γ_1 . For **negative pairs** $(u, v') \in N$, since our primary goal is to push $reg_{v'}$ outside of reg_u , it is sufficient to use the boundary dissimilarity $d_{bd}(reg_u, reg_{v'})$ rather than the energy $E(u, v')$. A threshold γ_2 is used to regulate how far $reg_{v'}$ is pushed from reg_u .

4 EVALUATION

Our experiments aim to address two questions: **(1)** How effectively do our methods capture hierarchical relationships? and **(2)** Can they generalize to tasks involving more than hierarchies?

We evaluate hierarchical relationship modeling using transitive DAGs (Section 4.1). To assess generalization, we test on *ontologies* (see Appendix E for a formal definition), which extend pure hierarchies by incorporating logical operations like conjunction (\sqcap) and existential quantifiers ($\exists r$). Ontologies contain ‘‘SubclassOf’’ (\sqsubseteq) as a fundamental and ubiquitous relation, representing hierarchical structures. This makes ontologies ideal for evaluating beyond pure hierarchy modeling. Specifically, ontologies enable testing of: **(a)** Complex inferences tasks beyond transitive closure (Section 4.2); and **(b)** Link prediction across different, usually non-SubclassOf relations (Section 4.3). Due to space limitations, additional results and detailed experimental settings are provided in Appendix D.

Table 2: F1 score (%) on Mammal, WordNet noun, MCG, and Hearst. Results with * are coming from Yu et al. (2024).

Method	Mammal		Noun		MCG		Hearst		
	d=2	d=5	d=5	d=10	d=5	d=10	d=5	d=10	
τ Box	29.0	33.5	30.5	31.5	43.9	50.3	39.7	43.7	
OE	25.4	31.0	28.8	30.8	36.3	46.6	34.6	40.7	
ELBE (box baseline)	30.3	36.8	30.7	31.8	48.4	55.5	41.6	46.8	
ELEM (ball baseline)	27.7	28.8	28.6	29.5	35.7	38.6	34.6	36.7	
EntailmentCone*	54.4	56.3	29.2	32.1	25.3	25.5	22.6	23.7	
ShadowCone*	(Umbral-half)	57.7	69.4	45.2	52.2	36.8	40.1	32.8	32.6
	(Penumbral-half)	52.8	67.8	44.6	51.7	35.0	37.6	26.8	28.4
RegD	(box)	64.9	71.6	53.8	51.3	50.7	58.5	42.8	49.6
	(ball)	62.7	71.8	58.4	59.1	44.9	46.8	37.7	37.7

4.1 INFERENCE OVER DAG

Benchmark Following Yu et al. (2024), we evaluate our method on four real-world datasets consisting of Is-A relations: MCG Wang et al. (2015); Wu et al. (2012), Hearst patterns Hearst (1992), the WordNet Fellbaum (1998) noun taxonomy, and its mammal subgraph. All models are trained exclusively on *basic edges*, which are edges not implied transitively by other edges in the graph. For validation and testing, we use the same sets as in Yu et al. (2024), consisting of 5% of *non-basic (inferred)* edges, ensuring a fair comparison. The hyperparameter settings are provided in Appendix D.1. We exclude non-basic edges from training since they can be transitively derived from basic edges. Including them would artificially inflate performance metrics without properly evaluating the embeddings’ ability to capture hierarchical structures. For completeness, results for non-basic cases are provided in Appendix D.3.

Baselines We compare our method RegD with (i) hyperbolic approaches such as EntailmentCone Ganea et al. (2018b) and ShadowCone Yu et al. (2024), which is the latest method with the state-of-the-art performance; (ii) region-based methods like OrderEmbedding Bordes et al. (2013), and tBox Boratko et al. (2021). We also compare with the ontology embedding methods, ELBE Peng et al. (2022) and ELEM Kulmanov et al. (2019), which can be considered as the baseline approaches embedding the DAG as boxes or balls, respectively. We use F1-scores as in previous studies.

Results The performance comparison across different DAGs is shown in Table 2. RegD achieved the best performance on all four datasets. Notably, the box variant consistently outperformed the ball variant in most cases, which might be because boxes contain more parameters than balls when embedded in the same dimensional space. Interestingly, region-based methods outperformed hyperbolic methods on the MCG and Hearst datasets. However, on the Noun and mammal dataset, hyperbolic methods performed better. Nevertheless, our method performed consistently well in both cases, as it can adjust the hyperbolic component by setting different λ values in Equation (7). The results of the ablation study are presented in Appendix D.2.

4.2 INFERENCE AND LINK PREDICTION OVER ONTOLOGIES

Benchmark We utilize three normalized biomedical ontologies: GALEN Rector et al. (1996), Gene Ontology (GO) Ashburner et al. (2000), and Anatomy (Uberon) Mungall et al. (2012). As in Jackermeier et al. (2024), we use the entire ontology for training, and the complete set of inferred class subsumptions for testing. Those subsumptions can be regarded as partial order pairs $u \prec v$. Evaluation is performed using 1,000 subsumptions randomly sampled from the test set. Similar to inference over DAG, negative samples are generated by randomly replacing the child of each positive pair 10 times.

Baselines We focus on the most representative ontology embedding methods: ELBE Peng et al. (2022) and ELEM Kulmanov et al. (2019), as well as their enhanced versions incorporating RegD or τ Box. Other hierarchy embedding methods are excluded from our tests due to their incompatibility

Table 3: F1 score (%) for the inference task.

Method	GALEN		GO		ANATOMY	
	d=5	d=10	d=5	d=10	d=5	d=10
ELBE	20.7	21.2	36.9	42.4	43.1	43.0
+ τ Box	20.8	20.7	32.2	34.7	42.2	47.2
+ RegD	25.2	25.8	50.0	50.5	58.7	62.5
ELEM	16.9	17.3	23.5	27.4	34.6	38.7
+ RegD	19.2	18.8	36.4	40.0	52.5	55.5

Table 4: F1 score (%) for the prediction task.

Method	GALEN		GO		ANATOMY	
	d=5	d=10	d=5	d=10	d=5	d=10
ELBE	21.0	24.2	32.8	37.9	25.1	25.5
+ τ Box	18.4	19.5	24.0	29.3	25.6	22.9
+ RegD	20.6	21.0	37.1	44.1	41.4	45.3
ELEM	16.7	16.6	54.5	54.2	23.1	26.0
+ RegD	16.8	18.0	60.3	61.4	21.7	21.9

with ontology embeddings. For example, OE and EntailmentCone utilizes cones as embedding objects, which cannot be directly integrated with ELBE or ELEM for ontology tasks. Details of the integration are provided in Appendix E.1.

Results The results are summarized in Tables 3. We can see that RegD yields consistent improvements across all ontologies for [inference](#) tasks. Specifically, [it gains an F1](#) score increase of more than 45% with ELBE method on the ANATOMY ontology. Conversely, the τ Box plugin consistently reduces performance across nearly all test cases, underscoring its limited applicability to tasks involving more than hierarchies.

4.3 LINK PREDICTION OVER ONTOLOGIES

We use the same baselines and datasets as described in Section 4.2. However, in this prediction task, we partition the original ontologies directly into 80% for training, 10% for validation, and 10% for testing as in Jackermeier et al. (2024). For the link prediction task, we focus on specific parts of the validation and testing sets, represented as $\exists r.B \prec ?A$, where A and B are concept names and r is a role. This setup is equivalent to link prediction tasks $(?A, r, B)$ in knowledge graphs if we regard A , B , and r as the head entity, tail entity, and relation, respectively.

Results Table 3 summarizes the results. RegD shows mixed results: while it generally improves performance, it decreases scores on the GALEN ontology and ANATOMY ontology with ELEM. This degradation likely occurs in challenging prediction cases where all methods perform poorly. Nevertheless, RegD achieves significant improvements in other cases, notably increasing F1 score by 77.6% with ELBE on the ANATOMY ontology. In contrast, the τ Box plugin consistently reduces performance across almost all test cases.

5 CONCLUSION

We introduced a framework RegD for low-dimensional embeddings of hierarchies, leveraging two dissimilarity metrics between regions. Our method, applicable to regions in the Euclidean space, demonstrates versatility and has the potential for a wide range of tasks involving data beyond hierarchies. Additionally, we showed that our approach achieves comparable embedding performance to hyperbolic methods while being significantly simpler to implement.

For future work, we are interested in integrating our method with other approaches based on hyperbolic spaces. For instance, Hyperbolic Neural Networks Ganea et al. (2018a) currently depend on intricate manifold operations, such as parallel transport and [maps between manifold and tangent spaces](#), to perform matrix multiplications and vector additions. In contrast, our framework enables these computations to be carried out more directly through the parameter space, [which could eliminate the need for such complex manifold operations and thus simplify the implementation](#). Another promising direction for future work is to investigate replacing existing hyperbolic embedding components in related methods with our approach, including recent studies that couple large language models with hyperbolic embeddings to learn semantic hierarchies He et al. (2024b), [which can be extended from atomic concept to complex ones by integrating the ontology embeddings as in Section 4.2](#). Also, we are interested in generalizing our framework to support a wider variety of

486 region types—beyond the balls and boxes considered here—so that it can be better adapted to the
487 requirements of diverse downstream tasks.

488
489 **Reproducibility statement** All code and data are publicly available at [https://anonymous.](https://anonymous.4open.science/r/RegD-F4E3)
490 [4open.science/r/RegD-F4E3](https://anonymous.4open.science/r/RegD-F4E3), along with clear instructions on environment configuration
491 and hyperparameter settings to enable full reproduction of our results.

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677 A PROOFS

678 A.1 THEOREM 1

679 *Proof of Theorem 1.* We begin by proving the result for balls and addressing each item as follows:
680

- 681
682 1. Let $reg_1 = ball(\mathbf{c}_1, r_1)$ and $reg_2 = ball(\mathbf{c}_2, r_2)$. For any ball $ball(\mathbf{c}', r') \subseteq ball(\mathbf{c}_2, r_2)$
683 with $r' \leq 0.5 \cdot r_1$, we must have:

$$684 \|\mathbf{c}_1 - \mathbf{c}'\|_p^p + |r_1 - r'|^p > (0.5 \cdot r_1)^p.$$

685
686 Therefore, we have:

$$687 d_{\text{dep}}(reg_1, ball(\mathbf{c}', r')) = \frac{\|\mathbf{c}_1 - \mathbf{c}'\|_p^p + |r_1 - r'|^p}{f(reg_1)f(ball(\mathbf{c}', r'))} > \frac{(0.5 \cdot r_1)^p}{f(reg_1)f(ball(\mathbf{c}', r'))}.$$

688 Thus, when:

$$689 f(ball(\mathbf{c}', r')) < \epsilon := \frac{(0.5 \cdot r_1)^p}{f(reg_1)[d_{\text{dep}}(reg_1, reg_2) + \Delta]},$$

690 we can guarantee that $d_{\text{dep}}(reg_1, ball(\mathbf{c}', r')) > d_{\text{dep}}(reg_1, reg_2) + \Delta$.

691 Note that by our assumption, we have:

$$692 \lim_{reg \rightarrow \emptyset} f(reg) = 0.$$

693 Therefore, there exists a $\delta > 0$ such that when $r < \delta$, we have $f(reg) \leq \epsilon$ for any region
694 $reg = ball(\mathbf{c}, r)$. In conclusion, $r_0 = \min\{\delta, 0.5 \cdot r_1\}$ satisfies the required condition.
695
696
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698
699
700
701

- 702 2. Let $reg = ball(\mathbf{c}, r)$. For any $n, M > 0$, we can select n distinct vectors $\mathbf{c}_1, \dots, \mathbf{c}_n \in$
 703 $ball(\mathbf{c}, 0.5 \cdot r)$ such that:

$$704 \quad \|\mathbf{c}_i - \mathbf{c}_j\|_p^p > \delta > 0 \quad \text{for some } \delta > 0.$$

705
 706 Similarly to item 1, we can choose r_i small enough such that for any ball $ball(\mathbf{c}_i, r_i)$, we
 707 have:

$$708 \quad f(ball(\mathbf{c}_i, r_i)) < \left(\frac{\delta}{M}\right)^{0.5}.$$

709 Thus, we obtain:

$$710 \quad d_{\text{dep}}(ball(\mathbf{c}_i, r_i), ball(\mathbf{c}_j, r_j)) > \frac{\delta}{f(ball(\mathbf{c}_i, r_i))f(ball(\mathbf{c}_j, r_j))} \geq M.$$

711 This concludes the proof of item 2.

712 The proof for the case of boxes follows the same reasoning, with the radius r replaced by the offset \mathbf{o}
 713 or its norm $\|\mathbf{o}\|$. \square

714 A.2 PROPOSITION 1

715 *Proof of Proposition 1.* Recall that when the curvature is -1 , the distance in the hyperbolic space
 716 (half-plane model) is given by:

$$717 \quad d_k(\mathbf{x}, \mathbf{y}) = \text{arcosh} \left(1 + \frac{\|\mathbf{x} - \mathbf{y}\|_2^2}{2\mathbf{x}_n \mathbf{y}_n} \right).$$

718 Then, the distance induced by the function F is of the form:

$$719 \quad d_{\mathbb{B}^n}^\#(ball(\mathbf{c}, r), ball'(\mathbf{c}', r')) = \text{arcosh} \left(1 + \frac{\|\mathbf{c} - \mathbf{c}'\|_2^2 + (r - r')^2}{2rr'} \right).$$

720 This coincides with the depth dissimilarity in Example 1 when $p = 2$, $g(x) = \text{arcosh}(x + 1)$, and
 721 $f(ball(\mathbf{c}, r)) = \sqrt{2}r$. This completes the proof. \square

722 A.3 PROPOSITION 2

723 *Proof of Proposition 2.* This proposition follows directly from Proposition 1. The function $h(x) =$
 724 $\text{arcosh}(x + 1)$ is an increasing bijection from $\mathbb{R}_{\geq 0}$ to $\mathbb{R}_{\geq 0}$. Thus, for any $x, x' \geq 0$, we have:

$$725 \quad x \leq x' \iff h^{-1}(x) \leq h^{-1}(x').$$

726 By the assumption of this proposition, $d_{\text{dep}}(\cdot, \cdot) = k \cdot h^{-1}(d_{\mathbb{H}^n}(\cdot, \cdot))$, where $k > 0$. Therefore, for any
 727 points $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4 \in \mathbb{H}^n$, we have:

$$728 \quad d_{\mathbb{H}^n}(\mathbf{x}_1, \mathbf{x}_2) < d_{\mathbb{H}^n}(\mathbf{x}_3, \mathbf{x}_4)$$

729 if and only if

$$730 \quad d_{\text{dep}}(F^{-1}(\mathbf{x}_1), F^{-1}(\mathbf{x}_2)) < d_{\text{dep}}(F^{-1}(\mathbf{x}_3), F^{-1}(\mathbf{x}_4)).$$

731 \square

732 A.4 PROPOSITION 3

733 *Proof of Proposition 3.* We prove each item one-by-one:

- 734 1. By definition, we have $d_{\text{bd}}(reg_1, reg_2) \leq 0$ if and only if $reg_1 \subseteq reg_2$. Next, we focus on
 735 the case $d_{\text{bd}}(reg_1, reg_2) = 0$.

Note that if $d_{\text{bd}}(reg_1, reg_2) = 0$, we must have $reg_1 \subseteq reg_2$. Otherwise, we have

$$736 \quad d_{\text{bd}}(reg_1, reg_2) = \max_{\mathbf{x}_2 \in reg_2 \setminus reg_1} \{d(reg_1, \mathbf{x}_2)\} = 0$$

Therefore, for any $\mathbf{x}_2 \in \text{reg}_2$, we have $d(\text{reg}_1, \mathbf{x}_2) = 0$, therefore $\mathbf{x}_2 \subseteq \text{reg}_1$ (assuming reg_1 is a closed set). Contradiction!

Since $\text{reg}_1 \subseteq \text{reg}_2$, we have

$$d_{\text{bd}}(\text{reg}_1, \text{reg}_2) = \max_{\mathbf{x}_2 \in \text{reg}_2} \{-d(\text{reg}_1^c, \mathbf{x}_2)\} = 0.$$

Therefore, there must exist $\mathbf{x}_2 \in \text{reg}_2$ such that $d(\text{reg}_1^c, \mathbf{x}_2) = 0$, and thus $\mathbf{x}_2 \in \text{reg}_1^c$. Since we have $\mathbf{x}_2 \subseteq \text{reg}_2 \subseteq \text{reg}_1$, therefore, $\mathbf{x}_2 \in \partial(\text{reg}_1)$. Similarly, since $\mathbf{x}_2 \subseteq \text{reg}_1^c \subseteq \text{reg}_2^c$ and $\mathbf{x}_2 \in \text{reg}_2$, we also have $\mathbf{x}_2 \in \partial(\text{reg}_2)$. This finishes the proof of the first case.

2. By assumption, we have

$$d_{\text{bd}}(\text{reg}_1, \text{reg}_2) = \max_{\mathbf{x}_2 \in \text{reg}_2} \{-d(\text{reg}_1^c, \mathbf{x}_2)\}, \quad d_{\text{bd}}(\text{reg}_1, \text{reg}_2') = \max_{\mathbf{x}_2 \in \text{reg}_2'} \{-d(\text{reg}_1^c, \mathbf{x}_2)\}.$$

Since $\text{reg}_2' \subseteq \text{reg}_2$, of course we have

$$d_{\text{bd}}(\text{reg}_1, \text{reg}_2') \leq d_{\text{bd}}(\text{reg}_1, \text{reg}_2).$$

This finishes the proof of the second case.

□

A.5 GENERAL PARAMETERIZED REGIONS

A set of **parameterized regions** over Euclidean Space \mathbb{R}^n can be defined as all regions reg of the following form:

$$\text{reg}(\boldsymbol{\theta}) = \{\mathbf{x} \in \mathbb{R}^n : f_i(\mathbf{x}, \boldsymbol{\theta}) \leq 0, \quad \text{for } i = 1, \dots, n\}, \quad (9)$$

where f_1, \dots, f_n are given (differentiable) functions from the given space to \mathbb{R} and $\boldsymbol{\theta} = (\theta_1, \dots, \theta_m) \in \mathbb{R}^m$ is the m -dimensional parameter. Let \mathcal{R} denote a space of parameterized regions $\text{reg}(\boldsymbol{\theta})$ as in Equation 9, with $\boldsymbol{\theta} = (\theta_1, \dots, \theta_m) \in \mathbb{R}^m$. For simplicity, and without significant loss of generality, in this section, we assume that all parameterized regions spaces \mathcal{R} satisfies the following properties:

- **Volume-like parameter.** The last coordinate θ_m of $\boldsymbol{\theta}$ serves as a volume parameter such that $\theta_m > 0$ and $\lim_{\text{reg}(\boldsymbol{\theta}) \rightarrow \emptyset} \theta_m = 0$
- **Non-empty regions:** For any $\boldsymbol{\theta} \in \mathbb{R}^m$ with $\theta_m > 0$, the corresponding region $\text{reg}(\boldsymbol{\theta})$ is non-empty.
- **Uniqueness:** Two regions coincide if and only if their parameters are equal, i.e., $\text{reg}(\boldsymbol{\theta}) = \text{reg}(\boldsymbol{\theta}') \iff \boldsymbol{\theta} = \boldsymbol{\theta}'$.
- **Contractible:** For any parameter $\boldsymbol{\theta}$, there exists a sequence $\{\boldsymbol{\theta}^k = (\theta_1^k, \dots, \theta_m^k)\}_{k=0}^\infty$ such that $\boldsymbol{\theta}^0 = \boldsymbol{\theta}$, $\theta_m^k > 0$ for all $k \geq 0$, $\text{reg}(\boldsymbol{\theta}^{k+1}) \subset \text{reg}(\boldsymbol{\theta}^k)$ for all $k \geq 0$, and $\lim_{k \rightarrow \infty} \text{reg}(\boldsymbol{\theta}^k) = \emptyset$.

It is worth noting that the spaces of balls and boxes in Examples 1 and 2 satisfy all of the above properties.

Notably, the results established in Theorem 1 naturally generalize to other parameterized regions, with proofs following analogous arguments. The result for the general case is of the following form.

Theorem 2. Consider the parameterized region space \mathcal{R} satisfies assumptions above, and equipped with the depth dissimilarity as defined in Definition 1. The following properties hold:

1. For any $\text{reg}_1, \text{reg}_2 \in \mathcal{R}$ and any $\Delta > 0$, there exists reg_1 sufficiently small, such that

$$d_{\text{dep}}(\text{reg}_1, \text{reg}_2') > d_{\text{dep}}(\text{reg}_1, \text{reg}_2) + \Delta, \quad \forall \text{reg}_2' \subseteq \text{reg}_2.$$

2. For any $\text{reg} \in \mathcal{R}$, any integer n , and any $M > 0$, there exist subsets $\text{reg}_1, \dots, \text{reg}_n \subseteq \text{reg}$ such that for any distinct $i, j \in \{1, \dots, n\}$,

$$d_{\text{dep}}(\text{reg}_i, \text{reg}_j) > M.$$

810 *Outline of proof.* We sketch the main ideas, which closely follow the argument in the proof of
811 Theorem 1.

812 For the first statement, by selecting a sufficiently small subset $reg' \subseteq reg_2$, we can ensure that
813

$$814 \quad \|P(reg) - P(reg_1)\| > \delta$$

815 for some $\delta > 0$. Additionally, since $f(reg')$ can be made arbitrarily small as $reg' \rightarrow \emptyset$ (i.e.,
816 $\lim_{reg' \rightarrow \emptyset} f(reg') = 0$), we can make the numerator of the depth dissimilarity arbitrarily small while
817 keeping the denominator bounded below by a positive constant. Consequently, the depth dissimilarity
818 $d_{dep}(reg_1, reg')$ can be made arbitrarily large.

819 For the second statement, a similar argument applies: by choosing the subsets reg_1, \dots, reg_n to be
820 sufficiently small and mutually separated within reg , we can ensure that each $f(reg_i)$ is small enough
821 so that the depth dissimilarity between any pair (reg_i, reg_j) exceeds M .
822

□

823
824 Propositions 1 and 3 can also be extended to arbitrary regions as follows.

825 **Proposition 4.** Let \mathbb{H}^m denote the hyperbolic space with curvature -1 . Assume that \mathcal{R} is a collection
826 of parameterized regions satisfying the above assumptions, equipped with the depth dissimilarity
827 defined in Equation equation 1. Then the map $F: \mathcal{R} \rightarrow \mathbb{H}^m$ defined by $F(\theta) = \theta$ is a bijective
828 isometry between \mathcal{R} and \mathbb{H}^m when $p = 2$, $g(x) = \text{arcosh}(x + 1)$, and $f(reg(\theta)) = \sqrt{2}\theta_m$.
829

830 *Proof.* Under the given condition, the distance in the \mathbb{H}^{n+1} is given by:
831

$$832 \quad d_k(\mathbf{x}, \mathbf{y}) = \text{arcosh} \left(1 + \frac{\|\mathbf{x} - \mathbf{y}\|_2^2}{2\mathbf{x}_n \mathbf{y}_n} \right).$$

833 Then, the distance induced by the function F is of the form:
834

$$835 \quad d_{\mathcal{R}}^{\#}(reg(\theta), reg(\theta')) = \text{arcosh} \left(1 + \frac{\|\theta - \theta'\|_2^2}{2\theta_m \theta'_m} \right).$$

836 This coincides with the depth dissimilarity in Equation 1 when $p = 2$, $g(x) = \text{arcosh}(x + 1)$, and
837 $f(reg(\theta)) = \sqrt{2}\theta_m$.
838

839 **Proposition 5.** Following Proposition 4, let the depth dissimilarity d_{dep} be redefined by replacing g
840 to $g(x) = k \cdot x$ ($k > 0$). Then the map F retains the following monotonicity property: for any points
841 $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4 \in \mathbb{H}^n$, $d_{\mathbb{H}^n}(\mathbf{x}_1, \mathbf{x}_2) < d_{\mathbb{H}^n}(\mathbf{x}_3, \mathbf{x}_4)$ if and only if
842

$$843 \quad d_{dep}(F^{-1}(\mathbf{x}_1), F^{-1}(\mathbf{x}_2)) < d_{dep}(F^{-1}(\mathbf{x}_3), F^{-1}(\mathbf{x}_4)).$$

844 *Proof.* The proof is the same as the proof of Proposition 3 in Appendix A.4 because of the function
845 $h(x) = \text{arcosh}(x + 1)$ is an increasing bijection from $\mathbb{R}_{\geq 0}$ to $\mathbb{R}_{\geq 0}$.
846

□

847 B HYPERBOLIC BOUNDARY DISSIMILARITY FOR BALLS

848 A ball in \mathbb{R}^n can be mapped to a cone in the upper half-space $\mathbb{R}^n \times \mathbb{R}_{>0}$ via a mapping G . This
849 transformation is illustrated in Figure 4 for the case $n = 1$, where a ball $ball(0, 1)$ is mapped to a
850 cone with apex $(0, 1) \in \mathbb{R} \times \mathbb{R}_{>0}$. Note that the height of the cone corresponds to the radius of
851 the underlying ball. The upper half-space can be interpreted as the Poincaré half-plane model of
852 hyperbolic space.

853 Formally, we are considering a cone with a base as a ball $ball(\mathbf{c}, r)$ and a height $k > 0$, which can be
854 defined as:

$$855 \quad Cone(ball(\mathbf{c}, r), k) = \{(1-t)\mathbf{x} + t(\mathbf{c} + k\mathbf{e}_{n+1}) : \mathbf{x} \in ball(\mathbf{c}, r), t \in [0, 1]\},$$

856 where $\mathbf{e}_{n+1} = (0, \dots, 0, 1) \in \mathbb{R}^{n+1}$. The mapping G is defined by:
857

$$858 \quad G(ball(\mathbf{c}, r)) = Cone(ball(\mathbf{c}, r), r).$$

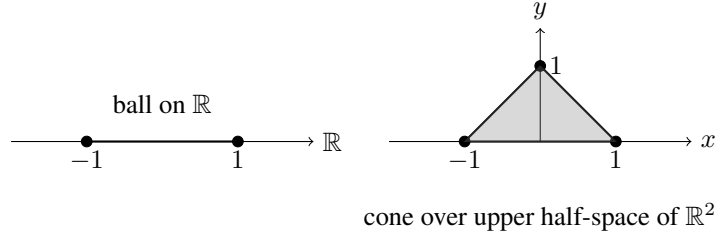


Figure 4: Mapping from balls to cones in the case of dimension 1.

The boundary dissimilarity between two cones in the Poincaré half-plane model (as shown on the right of Figure 4) can be defined as:

$$d_{\text{bd}}^{\text{cone}}(\text{Cone}_1, \text{Cone}_2) := \chi \cdot \min d_{\mathbb{H}}(\partial(\text{Cone}_1), \text{Apex}(\text{Cone}_1)),$$

where $\chi = -1$ if $\text{Cone}_2 \subseteq \text{Cone}_1$, and $\chi = 1$ otherwise. $\partial(\text{Cone}_1)$ denotes the boundary of Cone_1 , and $\text{Apex}(\text{Cone}_1)$ is the apex of Cone_1 , which is a single point.

Assuming the curvature is fixed at -1 (i.e., $k = 1$), we specialize Theorem 4.2 from Yu et al. (2024) by imposing the condition $\sinh(\sqrt{k}r) = 1$, from which we derive:

$$d_{\text{bd}}^{\text{cone}}(\text{Cone}_1(\text{ball}(\mathbf{c}_1, r_1), r_1), \text{Cone}_2(\text{ball}(\mathbf{c}_2, r_2), r_2)) = \text{arcsinh}\left(\frac{\|\mathbf{c}_1 - \mathbf{c}_2\| - r_1}{r_2}\right) + \text{arcsinh}(1),$$

where \mathbf{c}_i and r_i are the center and radius of the underlying balls corresponding to the cones.

This distance can be extended back to the context of balls, allowing the definition of a boundary dissimilarity between balls as:

$$d_{\text{bd}}^{\text{cone}}(\text{ball}_1(\mathbf{c}_1, r_1), \text{ball}_2(\mathbf{c}_2, r_2)) = \text{arcsinh}\left(\frac{\|\mathbf{c}_1 - \mathbf{c}_2\| - r_1}{r_2}\right) + \text{arcsinh}(1).$$

C POINCARÉ BALL MODELS

There exist multiple models \mathbb{H} that are isometric to each other. This work uses two such models, the Poincaré ball and the Poincaré half-space:

The **Poincaré ball** is given by

$$B^n = \{x \in \mathbb{R}^n : \|x\| < 1/\sqrt{k}\}.$$

Distances on B^n are defined as

$$d_k(x, y) = \frac{1}{\sqrt{k}} \text{arcosh}\left(1 + \frac{2k\|x - y\|^2}{(1 - k\|x\|^2)(1 - k\|y\|^2)}\right).$$

D EXPERIMENTS SETTING

D.1 HYPERPARAMETERS

Following the setup in Yu et al. (2024), we evaluated our models in dimensions 5 and 10. The weighting coefficient λ in Eq. 7 was selected from $\{0, 0.5, 1\}$, while the learning rate was tuned over $\{0.01, 0.005, 0.001, 0.0005\}$. For the small dataset of mammals, which contains approximately 1000 nodes, we choose batch sizes from $\{32, 64, 128\}$. For the remaining datasets, we opt for batch sizes from $\{1024, 2048, 8192\}$. For the depth dissimilarity, we tested $p \in \{1, 2\}$ as specified in Definition 2. The boundary dissimilarity margins in Eq. 4 were set to $\gamma_1 = 0.001$ and $\gamma_2 = 0$ for directed acyclic graph (DAG) embedding tasks. In ontology embedding experiments, both margins were set to zero.

For DAG experiments, as in Yu et al. (2024), we trained for 400 epochs on the mammal and noun datasets and 500 epochs on the MCG and Hearst datasets. For ontology embedding experiments, we

Table 5: F1 score (%) on Mammal, WordNet noun, MCG, and Hearst with best numbers **bolded**.

region	Options			Mammal		Noun		MCG		Hearst	
	λ	p	boundary dissimilarity	d=2	d=5	d=5	d=10	d=5	d=10	d=5	d=10
Box	0	-	d_{bd}	39.4	42.8	34.6	34.6	49.9	56.6	41.6	44.7
			d_{vol}	31.7	38.1	30.8	31.9	48.6	58.5	42.8	49.6
	> 0	1	d_{bd}	64.9	<u>71.6</u>	53.8	51.3	43.7	45.0	35.6	38.8
			d_{vol}	45.6	54.3	30.4	33.4	30.9	39.9	32.6	38.8
		2	d_{bd}	56.1	62.2	50.3	47.4	50.7	<u>57.4</u>	40.6	44.6
			d_{vol}	39.7	47.9	30.6	31.6	48.5	56.7	37.8	43.8
Ball	0	-	d_{bd}	42.8	55.5	39.6	42.5	43.9	46.7	37.7	37.1
			d_{bd}^{cone}	41.2	49.7	36.4	37.7	40.9	43.7	36.0	36.7
	> 0	1	d_{bd}	58.2	69.2	51.7	54.4	40.9	45.9	33.6	35.8
			d_{bd}^{cone}	57.9	65.3	52.3	54.7	36.8	41.7	31.6	34.6
		2	d_{bd}	62.5	71.8	58.4	59.1	41.7	45.8	34.8	37.7
			d_{bd}^{cone}	<u>62.7</u>	67.7	<u>54.3</u>	<u>55.1</u>	40.7	45.7	34.6	36.7

trained for 5000 epochs, following the protocol in the previous work Jackermeier et al. (2024) of ontology embedding.

All experiments were conducted on a system equipped with an AMD Ryzen Threadripper PRO 7965WX 24-core processor, 128GB of RAM, and an NVIDIA A6000 GPU with 48GB of VRAM, running Ubuntu 24.04.

D.2 DETAILED RESULTS

The detail results under different hyperparameter choices of λ , p and boundary dissimilarities are summarized in Table 5. Note that, when $\lambda = 0$, the depth dissimilarity component is absent from the energy function, and therefore, the choice of p , as a hyperparameter of depth dissimilarity, is not applicable.

From the results, it is evident that our boundary dissimilarity generally outperforms the specific boundary dissimilarities for boxes and balls (i.e., d_{vol} and d_{bd}^{cone}) in most cases. Furthermore, when using boxes as the embedding object, setting $p = 1$ yields better results than $p = 2$. However, for balls, $p = 2$ achieves superior performance.

For the mammal and noun datasets, using balls as the embedding object and incorporating the depth dissimilarity (i.e., $\lambda > 0$) in the energy function results in better performance. Conversely, for the MCG and Hearst datasets, the best performance is typically achieved when using boxes as the embedding region and setting $\lambda = 0$, effectively excluding the hyperbolic components. This observation aligns with our analysis in the main text.

It is worth noting, as shown in the seventh row of Table 5, that even under a small configuration range (i.e., with box and $\lambda \in \{0.5, 1\}$), our method outperforms existing approaches and exhibits only minimal performance gaps compared to the best results obtained with other configurations.

D.3 OTHER RESULTS

Including non-basic edges in training We evaluated the impact of including different percentages of transitive closure edges in the training set using the mammal dataset. The results, presented in Table 6, demonstrate that our method achieved overall superior performance compared to existing approaches. This was particularly evident when the dimension was 2, where our method outperformed all other approaches across all conditions except with 25% non-basic edges—and even then, our F1-score was only 0.2 lower than the best performer. Our method exhibited more stable performance characteristics, with F1-scores increasing gradually as we added non-basic edges to the training set. In contrast, the current state-of-the-art method, ShadowCone, showed sharp initial

Table 6: F1 score (%) on mammal sub-graph with best numbers **bolded**. Results with * are coming from Yu et al. (2024). For ShadowCone, only result of Umbral-half-space is reported as in Yu et al. (2024).

Non-basic-edge	Dimension = 2					Dimension = 5				
	0%	10%	25%	50%	90%	0%	10%	25%	50%	90%
Percentage										
GBC-box*	23.4	25.0	23.7	43.1	48.2	35.8	60.1	66.8	83.8	97.6
VBC-box*	20.1	26.1	31.0	33.3	34.7	30.9	43.1	58.6	74.9	69.3
τ Box	29.0	33.0	41.2	49.6	53.5	33.5	37.5	45.0	58.9	64.0
EntailmentCone*	54.4	61.0	71.0	66.5	73.1	56.3	<u>81.0</u>	<u>84.1</u>	83.6	82.9
ShadowCone*	57.7	<u>73.7</u>	77.4	<u>80.3</u>	79.0	69.4	81.1	83.7	88.5	<u>91.8</u>
Ours (box)	64.9	74.4	75.8	78.3	82.8	71.6	77.8	83.2	87.6	87.0
Ours (ball)	<u>62.7</u>	68.3	<u>77.2</u>	84.1	88.6	71.8	74.5	84.4	<u>88.4</u>	90.2

Table 7: Average and standard deviation (Std) of 10 random runs of F1 score (%) on Mammal, WordNet noun, MCG, and Hearst.

RegD		Mammal		Noun		MCG		Hearst	
		d=2	d=5	d=5	d=10	d=5	d=10	d=5	d=10
fixed seed	box	64.9	71.6	53.8	51.3	50.7	58.5	42.8	49.6
	ball	62.7	71.8	58.4	59.1	44.9	46.8	37.7	37.7
average (\pm std)	box	63.00 (± 2.01)	69.65 (± 3.14)	52.98 (± 1.00)	49.33 (± 1.12)	50.49 (± 0.44)	57.71 (± 0.41)	42.70 (± 0.50)	48.72 (± 0.12)
	ball	56.70 (± 4.91)	66.76 (± 2.91)	51.63 (± 1.52)	59.31 (± 2.29)	44.09 (± 0.55)	46.35 (± 0.37)	37.24 (± 0.37)	37.11 (± 0.47)

improvements followed by diminishing returns. Specifically, when increasing non-basic edges from 0% to 10%, ShadowCone’s F1-scores jumped dramatically (increasing by 16.0 and 11.7 points for dimensions 2 and 5, respectively). However, further increases from 10% to 25% yielded much smaller improvements (3.7 and 2.6 points for dimensions 2 and 5, respectively).

Repeatness The main experiments presented in this paper were conducted using a fixed random seed, following established practices in previous works Yu et al. (2024); Ganea et al. (2018b). To assess the repeatability and robustness of our results, we conducted 10 independent experimental runs on each of the four datasets. The average performance and standard deviation are reported in Table 7, while the outcomes of individual runs are summarized in Figure 5. These results demonstrate that our method exhibits considerable stability, particularly on the MCG and Hearst datasets. Compared to the main results obtained with a fixed random seed, the overall average performance remains very close, with only a few exceptions:

1. In certain cases—such as using balls on the Mammal dataset with $d = 2$ and on the Noun dataset with $d = 5$ —performance is slightly lower, though still superior to that of other baseline methods.
2. In some settings, performance is even improved on average, for example, when using balls on the Noun dataset with $d = 10$.

These results indicate that the proposed method is robust across different random seeds, with consistent performance across most settings.

Impact of λ In Table 5, we evaluate the performance of $\lambda = 0, 0.5, \text{ and } 1$, and report results for both $\lambda = 0$ and $\lambda > 0$. To provide a more detailed analysis, Table 8 presents additional experiments with λ ranging from 0 to 1 in increments of 0.1, using the mammal dataset (dim = 2, box embedding).

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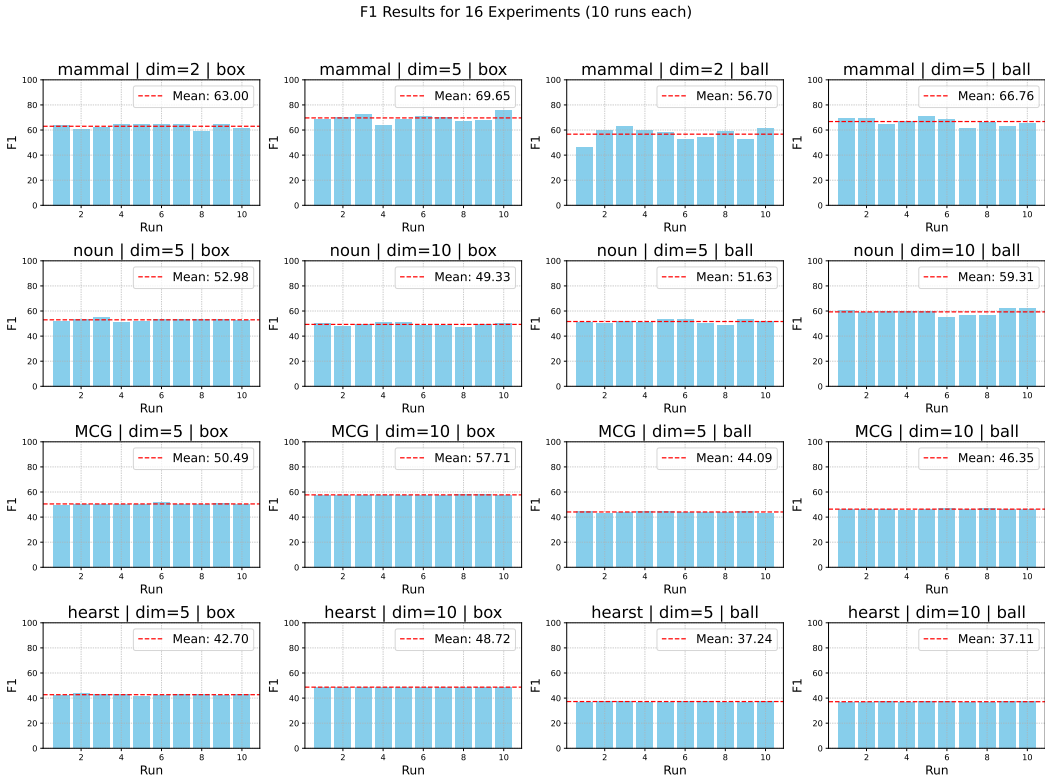


Figure 5: All F1 scores of 10 random runs on Mammal, WordNet noun, MCG, and Hearst.

The results suggest that the impact of λ may not follow a clear or consistent trend, and the optimal value of λ can vary significantly across different settings. For instance, in this dataset, larger values of λ generally lead to higher F1 scores compared to smaller ones. However, the relationship is not strictly monotonic—an increase in λ does not always result in improved performance.

	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
F1 (avg)	42.70	50.92	57.42	56.07	57.03	64.43	62.46	62.83	66.56	62.80	65.30
(\pm std)	(± 7.07)	(± 5.44)	(± 5.46)	(± 4.87)	(± 5.62)	(± 4.61)	(± 3.23)	(± 2.11)	(± 2.33)	(± 2.47)	(± 2.08)

Table 8: F1 scores with standard deviations for different λ values on the mammal dataset (dim=2, using box).

E ONTOLOGIES

Ontologies use sets of statements (axioms) about concepts (unary predicates) and roles (binary predicates) for knowledge representation and reasoning. We focus on \mathcal{EL} -ontologies, which strike a good balance between expressivity and reasoning efficiency, making them widely applicable Baader & Gil (2024).

Let $N_C = \{A, B, \dots\}$, $N_R = \{r, t, \dots\}$, and $N_I = \{a, b, \dots\}$ be pairwise disjoint sets of *concept names* (also called *atomic concepts*), *role names*, and *individual names*, respectively. \mathcal{EL} -concepts are recursively defined from atomic concepts, roles, and individuals as follows:

$$\top \mid \perp \mid A \mid C \sqcap D \mid \exists r.C \mid \{a\}$$

An \mathcal{EL} -ontology is a finite set of TBox axioms of the form

$$C \sqsubseteq D.$$

Note that here \sqsubseteq denotes ‘‘SubclassOf’’, which is a transitive relation that can be considered a partial order \prec by rewriting it as:

$$C \sqsubseteq D \Leftrightarrow D \prec C.$$

Example 4. From atomic concepts *Father*, *Child*, *Male*, ... and the role *hasParent*, we can construct a small family ontology consisting of two TBox axioms:

$$\textit{Father} \sqsubseteq \textit{Male} \sqcap \textit{Parent}, \quad \textit{Child} \sqsubseteq \exists \textit{hasParent}.\textit{Father}.$$

An interpretation $\mathcal{I} = (\Delta^{\mathcal{I}}, \cdot^{\mathcal{I}})$ consists of a non-empty set $\Delta^{\mathcal{I}}$ and a function $\cdot^{\mathcal{I}}$ that maps each $A \in \mathbb{N}_{\mathcal{C}}$ to $A^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}}$, and each $r \in \mathbb{N}_{\mathcal{R}}$ to $r^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}} \times \Delta^{\mathcal{I}}$, where $\perp^{\mathcal{I}} = \emptyset$ and $\top^{\mathcal{I}} = \Delta^{\mathcal{I}}$. The function $\cdot^{\mathcal{I}}$ is extended to any \mathcal{EL} -concepts as follows:

$$(C \sqcap D)^{\mathcal{I}} = C^{\mathcal{I}} \cap D^{\mathcal{I}}, \quad (10)$$

$$(\exists r.C)^{\mathcal{I}} = \{a \in \Delta^{\mathcal{I}} \mid \exists b \in C^{\mathcal{I}} : (a, b) \in r^{\mathcal{I}}\}. \quad (11)$$

An interpretation \mathcal{I} satisfies a TBox axiom $X \sqsubseteq Y$ if $X^{\mathcal{I}} \subseteq Y^{\mathcal{I}}$ for X and Y being either two concepts or two role names, or X being a role chain and Y being a role name. An ontology \mathcal{O} entails an axiom $C \sqsubseteq D$, written

$$\mathcal{O} \models C \sqsubseteq D \quad (\text{i.e., } \mathcal{O} \models D \prec C),$$

if $C \sqsubseteq D$ is satisfied by all models of \mathcal{O} . Ontologies can infer much more complex patterns than the transitive closure, as shown by the following example.

Example 5. In an ontology, suppose that in a group X , all members are both a man and a parent. That is, $X \sqsubseteq \textit{man}$ and $X \sqsubseteq \textit{parent}$ in the ontology. Moreover, *man* and *parent* together imply *father* (formally, $\textit{man} \sqcap \textit{parent} \sqsubseteq \textit{father}$ in the ontology). From this, we can infer that the group X is a *father*, which is not derivable from the transitive closure.

E.1 ONTOLOGY EMBEDDING METHODS

Implementation of ELBE and ELEM over DAG As discussed in the main text, the ontology embedding methods ELBE and ELEM can be adapted to serve as baseline methods for embedding DAGs using boxes and balls, respectively. Specifically, for a pair of nodes (u, v) , the energy function used during training is defined as follows:

1. **ELBE:** Nodes u and v are embedded as boxes \textit{box}_u and \textit{box}_v , respectively. The energy function is given by:

$$E(u, v) = \|\max\{\|\mathbf{c}_u - \mathbf{c}_v\| + \mathbf{o}_v - \mathbf{o}_u, \mathbf{0}\}\|,$$

where \mathbf{c}_u and \mathbf{c}_v denote the center vectors of the boxes, and \mathbf{o}_u and \mathbf{o}_v denote the offsets of the boxes.

2. **ELEM:** Nodes u and v are embedded as balls \textit{ball}_u and \textit{ball}_v , respectively. The energy function is defined as:

$$E(u, v) = \max\{\|\mathbf{c}_u - \mathbf{c}_v\| + r_v - r_u, \mathbf{0}\},$$

where \mathbf{c}_u and \mathbf{c}_v represent the centers of the balls, and r_u and r_v represent their radii.

Note that the original ELEM method includes a regularization term that enforces the norms $\|\mathbf{c}_u\|$ and $\|\mathbf{c}_v\|$ to be close to 1. However, for the DAG case, we omit this regularization primarily applies to scenarios involving relation embeddings, such as axioms of the form $A \sqsubseteq \exists r.B$ or $\exists r.B \sqsubseteq A$, as in the KGE methods TransE Bordes et al. (2013).

Integration of ELBE and ELEM with RegD and τ Box ELBE and ELEM are embedding approaches for normalized \mathcal{EL} -ontologies, which consist of four types of axioms $C \sqsubseteq D$:

$$A \sqsubseteq B, \quad A \sqcap B \sqsubseteq B', \quad A \sqsubseteq \exists r.B, \quad \exists r.B \sqsubseteq A.$$

ELBE embeds each atomic concept A as a box $\textit{box}(A) \subseteq \mathbb{R}^n$ and maps complex concepts like $\exists r.B$ to a new box obtained by translating $\textit{box}(B)$ by a vector $\mathbf{v}_r \in \mathbb{R}^n$:

$$\textit{box}(\exists r.B) = \{\mathbf{x} - \mathbf{v}_r \mid \mathbf{x} \in \textit{box}(B)\}$$

ELEM employs a similar approach but uses balls instead of boxes. The key differences between ELBE and ELEM are as follows:

- 1134 1. ELEM includes a regularization term, similar to TransE, to constrain the norm of the center
 1135 of each ball to be close to 1.
 1136
 1137 2. ELBE handles conjunctions more effectively, as the intersection of two boxes is still a
 1138 box. This allows it to define $box(A \sqcap B)$ as $box(A) \cap box(B)$. In contrast, ELEM, which
 1139 uses balls, cannot handle intersections directly and must use specialized mechanisms to
 1140 approximate satisfaction of the axiom $A \sqcap B \sqsubseteq B'$.

1141 To integrate RegD and τ Box into ELBE or ELEM, it suffices to replace their energy function for
 1142 axioms $C \sqsubseteq D$ with the corresponding energy function from RegD or τ Box. However, ELBE and
 1143 ELEM handle negative samples differently, using a loss function of the form:

$$1144 \mathcal{L} = \sum_{(C,D) \in P} E(D,C) + \sum_{(C',D') \in N} (\gamma - E(D',C')).$$

1147 When integrating with RegD, this loss function should also be replaced with the one defined in
 1148 Section 3.3.

1149
 1150 **Result of prediction task by ranking-based metrics** The evaluation results for the prediction task
 1151 on ontologies are presented in Table 9. RegD shows consistent improvements for both ELEM and
 1152 ELBE across most cases. The gains are particularly notable for the GO and ANATOMY ontologies,
 1153 where the H@100 score increases from 0 to 0.26. In contrast, performance on the GALEN ontology
 1154 remains low for both variants (with or without RegD), likely due to the inherent complexity of
 1155 GALEN. This suggests that more advanced methods may be required to effectively model such
 1156 complex structures.

1157 F THE USE OF LLMs

1158 LLMs have been employed solely to assist with polishing the writing. All content was originally
 1159 written by the authors and subsequently refined by LLMs to improve readability, clarity, and to correct
 1160 grammatical errors or typographical mistakes.
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Table 9: Prediction task

Dataset	Method	H@1	H@10	H@100	Medain	MRR	MR	AUC
GALEN (d=5)	ELBE	0	0	0	7831	0	9044	0.61
	+ RegD	0	0	0.02	9506	0	10056	0.57
	ELEM	0	0.01	0.04	8843	0	9361	0.60
	+ RegD	0	0	0.02	10122	0	10531	0.55
GALEN (d=10)	ELBE	0	0	0	8812	0	9595	0.59
	+ RegD	0	0.01	0.02	8966	0	9729	0.58
	ELEM	0	0	0.03	8856	0	9534	0.59
	+ RegD	0	0.01	0.03	9996	0	10441	0.55
GO (d=5)	ELBE	0	0	0	14058	0	17231	0.62
	+ RegD	0	0.10	0.19	8466	0.02	14376	0.69
	ELEM	0	0	0.01	19666	0	19813	0.57
	+ RegD	0	0.01	0.03	15440	0	17983	0.61
GO (d=10)	ELBE	0	0	0	18926	0	19656	0.57
	+ RegD	0	0.17	0.26	7785	0.04	14244	0.69
	ELEM	0	0	0.01	19668	0	20543	0.55
	+ RegD	0	0.02	0.06	17194	0.01	19019	0.59
ANATOMY (d=5)	ELBE	0	0	0.01	19556	0	29528	0.72
	+ RegD	0	0.02	0.05	14317	0.01	25582	0.76
	ELEM	0	0.01	0.04	23437	0	32788	0.69
	+ RegD	0	0.04	0.14	8616	0.01	27272	0.74
ANATOMY (d=10)	ELBE	0	0	0.03	14955	0	25844	0.76
	+ RegD	0	0.05	0.13	10019	0.02	22215	0.79
	ELEM	0	0.01	0.06	14573	0	27010	0.75
	+ RegD	0	0.07	0.22	8066	0.03	27632	0.74