

Toward a Manifold-Preserving Temporal Graph Network in Hyperbolic Space

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Abstract

Hyperbolic geometry provides an ideal setting to represent the scale-free or hierarchical characteristics of an input graph naturally. Utilizing hyperbolic geometry for learning dynamic graph representation has gained a growing interest in recent years. However, the majority of hyperbolic-based approaches rely on tangent spaces to perform graph operations, which could distort the structure of the dynamic graph when the graph grows over time. To avoid the distortion in tangent space, we propose a Hyperbolic Manifold-Preserving Temporal Graph Network that works directly on the hyperbolic manifold. The model includes a graph convolution module for learning the spatial dependencies, an attention architecture for capturing the temporal properties, and a gated recurrent unit for extracting the spatio-temporal relationships. By evaluating on diverse real-world dynamic graphs, our model has achieved significant improvements in link prediction and new link prediction tasks, in comparison with other baselines.

1 Introduction

Many real-world complex networks [Leskovec *et al.*, 2007; Weber *et al.*, 2019] can be modeled as dynamic graphs. Learning representation of dynamic graph is a challenging but vital step to understand how the network interacts and evolves over time [Yang *et al.*, 2021]. Dynamic graphs, based on how the graphs undergo updates, can be categorized into two groups: continuous-time dynamic graphs [Rossi *et al.*, 2020] and discrete-time dynamic graphs [Xue *et al.*, 2021].

In a discrete-time dynamic graph, the changes in the graph presumably occur at separate time points and the graph structure at each time point is called a snapshot. Researchers have presented various methods for capturing the spatial and temporal dependencies of discrete dynamic graphs such as EvolveGCN [Pareja *et al.*, 2019] and VGRNN [Hajiramezanali *et al.*, 2020]. These two methods use the graph recurrent framework by incorporating a graph neural network, e.g., GCN [Kipf and Welling, 2016a] and a gate recurrent

unit, e.g., GRU [Cho *et al.*, 2014] to learn the embedding of a dynamic graph. Most of the discrete-based approaches are designed to work on the well-known Euclidean space. Alternatively, [Bronstein *et al.*, 2017] prove that many real-world graphs exhibit hierarchical structures and power-law distributions rather than uniform grid structures that best fit Euclidean space. In contrast to Euclidean geometry, hyperbolic geometry such as the Poincaré ball model or the Lorentz model, is more suitable for embedding scale-free and hierarchical graphs because of its exponential expansion property [Krioukov *et al.*, 2010].

Given the expressiveness of hyperbolic space in learning graph embedding, there has been an increasing interest in utilizing hyperbolic properties for learning representation of dynamic graph [Yang *et al.*, 2021; Li *et al.*, 2023]. Although hyperbolic methods have achieved state-of-the-art performance, their reliance on tangent space for graph operations is considered suboptimal. While the induced distance among two neighbor nodes' embedding on the hyperbolic manifold exhibits the hierarchical characteristic of the graph, it is not preserved after the mapping to the tangent space [Tuzel *et al.*, 2008]. In other words, the distance in tangent space is only a first-order approximation of the induced distance, which results in a distortion of the hierarchical structure of the given graph [Krioukov *et al.*, 2010; Lin *et al.*, 2023]. To address this issue, [Dai *et al.*, 2021] propose the H2H-GCN architecture which uses only the Lorentz model for graph operations, thus can avoid the distortion caused by projecting to tangent space. With the same purpose as H2H-GCN, DHGAT [Li *et al.*, 2023] designs spatio-temporal aggregate functions without depending on tangent space for representation learning in dynamic graphs.

In this work, we first give a detailed analysis of the distortion errors caused by the hyperbolic tangent space in representation learning for dynamic graphs. We show that the errors, which mainly come from the forward projection to tangent space and its reverse mapping, have lower bounds and increase as the graph evolves. Hence, to overcome the ineffectiveness of hyperbolic tangent space approaches, we propose a Hyperbolic Manifold-Preserving Temporal Graph Network (HMPTGN) that works directly on the hyperbolic manifold, rather than in tangent space. Our proposed model is centralized by a hyperbolic feature transformation which constrains the transformation matrix to be orthogonal to en-

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sure the node representation resides on the manifold. The hyperbolic feature transformation is then added to the standard graph neural network and gated recurrent unit to form the hyperbolic manifold-preserving graph neural network (HMPGNN) and hyperbolic manifold-preserving gated recurrent unit (HMPGRU) in the model, respectively. The HMPGNN is employed to capture spatial dependencies between nodes within the hyperbolic space, while the HMPGRU is used to extract the spatio-temporal representation of dynamic graph. An additional temporal attention component with manifold-preserving property (HMPTA) is integrated into the HMPTGN to extract the time-based relationship within a fixed-length historical window. We evaluate the performance of our model on two tasks, temporal link prediction task and new link prediction task on real-world dynamic graphs. The results demonstrate that our HMPTGN achieves significant improvements in comparison with other baselines, especially in new link prediction task.

2 Preliminaries

2.1 Problem Definition

A discrete-time dynamic graph is a collection of independent and complete snapshots $\{G_1, G_2, \dots, G_T\}$ sampled from a dynamic graph \mathcal{G} , where T is the number of snapshots and G_t is a snapshot at timestamp t . Each snapshot G_t has a particular node set V_t and a corresponding adjacency matrix A_t . Similar to [Pareja *et al.*, 2019; Yang *et al.*, 2021], our work is based on the graph recurrent framework which is defined as:

$$H_t = \psi(\phi(X_t, A_t), H_{t-1}), \quad (1)$$

where X_t are the initial features of the node set V_t and H_{t-1} is the latest historical state, ϕ is a graph neural network which aggregates local features and learns the node representation, and ψ is a recurrent model for learning the spatio-temporal properties. Possible choices for ϕ and ψ are GCN [Kipf and Welling, 2016a] and GRU [Cho *et al.*, 2014], respectively.

2.2 Hyperbolic Geometry in Graph Embedding

In general graph representation learning, the embedding H_t with Euclidean distance is used to characterize the graph structure. The extension of the learned embedding H_t to a hyperbolic space requires the definition of a Riemannian manifold (\mathcal{M}, g) , which is a differentiable manifold \mathcal{M} equipped with a Riemannian metric tensor g . Specifically, a hyperbolic space is a smooth Riemannian manifold with a constant negative curvature. Our work is built upon the *Poincaré ball model* due to its conformality and stability in learning graph embedding [Yang *et al.*, 2021].

Let $\|\cdot\|$ be the L2-norm. The Poincaré ball model of an n -dimensional hyperbolic space with constant negative curvature $-c$ ($c > 0$) is defined by the Riemannian manifold $\mathcal{B}_c^n = (\mathcal{H}^{n,c}, g^{\mathcal{H}^{n,c}})$, where $\mathcal{H}^{n,c} = \{x \in \mathbb{R}^n : c\|x\|^2 < 1\}$ is an open n -dimensional ball and $g^{\mathcal{H}^{n,c}}$ is the hyperbolic metric tensor which is conformal to the Euclidean metric tensor g^E :

$$g_x^{\mathcal{H}^{n,c}} = (\lambda_x^c)^2 g^E, \text{ where } \lambda_x^c = \frac{2}{1 - c\|x\|^2} \text{ and } g^E = \mathbf{I}_n. \quad (2)$$

The tangent space of a reference point x on \mathcal{B}_c^n is denoted as $\mathcal{T}_x \mathcal{B}_c^n$. Generally, the tangent space of a point on the Riemannian manifold is Euclidean which makes fundamental operations such as matrix-vector multiplication or vector addition trivial. However, to build a hyperbolic manifold-preserving method without the need of tangent space, we rely on further operations in the Poincaré ball model:

Möbius addition. This operation is proposed in the Möbius gyrovector spaces setting [Ungar, 2000]. Let $x, y \in \mathcal{B}_c^n$, the Möbius addition of x and y is defined as:

$$x \oplus_c y = \frac{(1 + 2c\langle x, y \rangle + c\|y\|^2)x + (1 - c\|x\|^2)y}{1 + 2c\langle x, y \rangle + c^2\|x\|^2\|y\|^2}. \quad (3)$$

When $c = 0$, one becomes the Euclidean addition of two vectors in \mathbb{R}^n .

Distance. The induced distance between two points on a manifold is the length of the shortest path between two points. In the Poincaré ball model \mathcal{B}_c^n , it is given by:

$$d_c(y, z) = \frac{2}{\sqrt{c}} \operatorname{arctanh}(\sqrt{c}\|(-y) \oplus_c z\|) \quad \forall y, z \in \mathcal{B}_c^n. \quad (4)$$

The hyperbolic distance d_c represents the geometric characteristic of the graph.

Isometric model for aggregation. Hyperbolic models such as HTGN [Yang *et al.*, 2021] and HGWaveNet [Bai *et al.*, 2023] project nodes to the tangent space $\mathcal{T}_x \mathcal{B}_c^n$ before conducting aggregate operations on them. To employ aggregate operations without relying on tangent space, we leverage the idea of using Einstein midpoint in the Klein model [Dai *et al.*, 2021; Li *et al.*, 2023]. In our aggregation operator, points in the Poincaré ball manifold are projected then aggregated in the Klein model and projected back to the original manifold. Let \mathcal{K}_c^n be the Klein model. The bijective connections between \mathcal{B}_c^n and \mathcal{K}_c^n , with the same dimension and curvature, are defined as:

$$p_{\mathcal{B}_c^n \rightarrow \mathcal{K}_c^n}(x) = \frac{2x}{1 + c\|x\|^2}, p_{\mathcal{K}_c^n \rightarrow \mathcal{B}_c^n}(k) = \frac{k}{1 + \sqrt{1 - c\|k\|^2}}, \quad (5)$$

where x is a node in the Poincaré ball model \mathcal{B}_c^n and k is a corresponding node in the Klein model \mathcal{K}_c^n .

3 Motivation

Most of the hyperbolic-based approaches depend on the tangent space projection which allows them to employ basic operations such as matrix-vector multiplication and vector addition. The mappings between the manifold \mathcal{B}_c^n and the tangent space $\mathcal{T}_x \mathcal{B}_c^n$ include the logarithmic map $\log_x^c : \mathcal{B}_c^n \rightarrow \mathcal{T}_x \mathcal{B}_c^n$ and the exponential map $\exp_x^c : \mathcal{T}_x \mathcal{B}_c^n \rightarrow \mathcal{B}_c^n$, which are defined as:

$$\log_x^c(y) = \frac{2}{\sqrt{c}\lambda_x^c} \operatorname{arctanh}(\sqrt{c}\|(-x) \oplus_c y\|) \frac{(-x) \oplus_c y}{\|(-x) \oplus_c y\|}, \quad (6)$$

$$\exp_x^c(y) = x \oplus_c \left(\tanh\left(\frac{\sqrt{c}\lambda_x^c\|y\|}{2}\right) \frac{y}{\sqrt{c}\|y\|} \right). \quad (7)$$

Note that the mappings cannot preserve the distances among nodes, which causes errors in the structure of the dynamic graph. In this section, we provide lower bounds of the

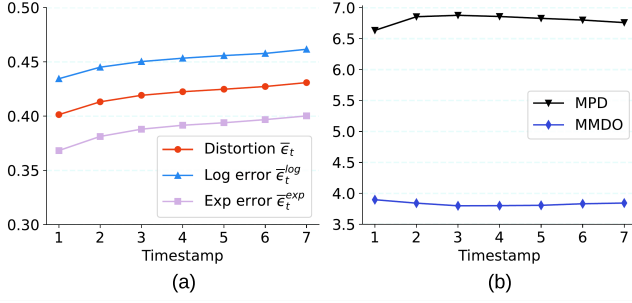


Figure 1: The errors caused by projecting to tangent space of HTGN on Disease dataset: (a) the average distortion, logarithmic and exponential errors; (b) the related measurements of MPD and MMDO.

projection errors and highlight that the errors increase over time in dynamic graph. Let y_t and z_t be two neighbor-node embeddings in the dynamic graph and x_t is a reference point, the two distortion errors for each mapping can be measured as follows.

Logarithmic error. Given three points $x_t, y_t, z_t \in \mathcal{B}_c^n$ at timestamp t , the logarithmic error ϵ_t^{\log} is defined as:

$$\epsilon_t^{\log}(y_t, z_t) = d_c(y_t, z_t) - \|\log_{x_t}^c(y_t) - \log_{x_t}^c(z_t)\|. \quad (8)$$

Exponential error. Given three points x_t, y_t, z_t at the timestamp t such that $y_t, z_t \in \mathcal{T}_{x_t}\mathcal{B}_c^n$ and $x_t \in \mathcal{B}_c^n$, the exponential error ϵ_t^{\exp} is defined as:

$$\epsilon_t^{\exp}(y_t, z_t) = d_c^{\exp}(y_t, z_t) - \|y_t - z_t\|. \quad (9)$$

The two errors measure the differences between the target distance in the Poincare ball and the distance in tangent space. Note that we use $d_c^{\exp}(y_t, z_t)$ for denoting the distance after the exponential map $d_c(\exp_{x_t}^c(y_t), \exp_{x_t}^c(z_t))$.

In general, the graph representation learning requires the distortion errors should be as close to 0 as possible [Tuzel *et al.*, 2008]. However, it is unlikely to occur in practice. The following theorem provides a lower bound of the logarithmic error:

Theorem 1 (Lower bound of logarithmic error). *Given three points $x_t, y_t, z_t \in \mathcal{B}_c^n$ at timestamp t and $\alpha = \max\{d_c(x_t, y_t), d_c(x_t, z_t)\}$, then*

$$\epsilon_t^{\log}(y_t, z_t) \geq d_c(y_t, z_t) - \alpha(1 - c\|x_t\|^2).$$

In the mapping $\mathcal{T}_{x_t}\mathcal{B}_c^n$, the term $c\|x_t\|^2$ is often fixed, so the lower bound of logarithmic error mainly depends on the pairwise distance $d_c(y_t, z_t)$ and the maximum distance of two points y_t, z_t to a reference point x_t . It can be verified that the lower bound is greater than 0 when $d_c(y_t, z_t)$ is greater than α . Similarly, we derive the lower bound of the exponential error as follows:

Theorem 2 (Lower bound of exponential error). *Given three points x_t, y_t, z_t at the timestamp t such that $y_t, z_t \in \mathcal{T}_{x_t}\mathcal{B}_c^n$ and $x_t \in \mathcal{B}_c^n$. Let $\alpha = \max\{d_c(x_t, \exp_{x_t}^c(y_t)), d_c(x_t, \exp_{x_t}^c(z_t))\}$, then*

$$\epsilon_t^{\exp}(y_t, z_t) \geq d_c^{\exp}(y_t, z_t) - \alpha(1 - c\|x_t\|^2).$$

In dynamic graph learning with hyperbolic geometry, we can assume that the graph is gradually scattered to fully leverage the expansive nature of hyperbolic space. This will lead to an increase in the distance d_c between any two nodes y_t and z_t . Hence, the lower bounds of two errors will also rise over time. To clarify our assumption, we conduct an experimental investigation of the HTGN on the Disease dataset [Bjørnstad *et al.*, 2002].

The Fig. 1a plots the $\bar{\epsilon}_t^{\log}$ and $\bar{\epsilon}_t^{\exp}$, which are computed as averaging the errors in Eq. (8) and Eq. (9) for each snapshot G_t . The distortion error $\bar{\epsilon}_t$ is denoted as the average of $\bar{\epsilon}_t^{\log}$ and $\bar{\epsilon}_t^{\exp}$. As the errors depend on the mean pairwise distance (MPD) among nodes in the hyperbolic space and the mean maximum distance to the origin point of the manifold (MMDO), we also give their plots in Fig. 1b. Because HTGN uses a fixed reference point, the term $(1 - c\|x_t\|)$ is constant. The MPD, correlating with the pairwise distance d_c in the error bound, slightly increases over time. Meanwhile, the MMDO, correlating with the term α in the error bound, gradually decreases. When the graph grows over time, the three error terms $\bar{\epsilon}_t$, $\bar{\epsilon}_t^{\log}$ and $\bar{\epsilon}_t^{\exp}$ grow linearly, which reduces the learning capability of HTGN in general.

4 Method

To avoid the distortion caused by tangent space, we propose the Hyperbolic Manifold-Preserving Temporal Graph Network (HMPTGN) that fully operates on the hyperbolic manifold. As illustrated in Fig. 2, our HMPTGN comprises three components: (i) HMPGNN - a graph neural network to capture spatial relationships within the hyperbolic space; (ii) HMPTA - a temporal attention mechanism to generate an informative historical state; (iii) HMPGRU - a recurrent unit to compute the output from the spatio-temporal features. Based on the graph recurrent framework [Yang *et al.*, 2021], each module is designed to learn relevant information to model the evolution of dynamic graphs. Moreover, by utilizing the Möbius addition, the Klein model, and the Poincaré linear transformation, the manifold-preserving property can be guaranteed in each of the three modules in HMPTGN.

4.1 Hyperbolic Manifold-Preserving Graph Neural Network

The HMPGNN module extends the standard message-passing framework from the Euclidean space to the hyperbolic manifold. As input graph snapshot $G_t(X_t, A_t)$ is represented in the Euclidean space, it is firstly needed to project to the hyperbolic space via Eq. (7). The resulting hyperbolic representation $G_t(X_t^{\mathcal{B}_c^n}, A_t)$ is then passed through L layers of the HMPGNN module. The l^{th} layer in HMPGNN receives the output $X_t^{l-1, \mathcal{B}_c^n}$ from the previous layer to produce the new node features X_t^{l, \mathcal{B}_c^n} . The initial hyperbolic representation of G_t is denoted as X_t^{0, \mathcal{B}_c^n} . As shown in Fig. 2, each l^{th} layer includes a feature transformation, a neighborhood aggregation, and a nonlinear activation.

Hyperbolic feature transformation. The feature transformation in Euclidean GCNs is a linear transformation based

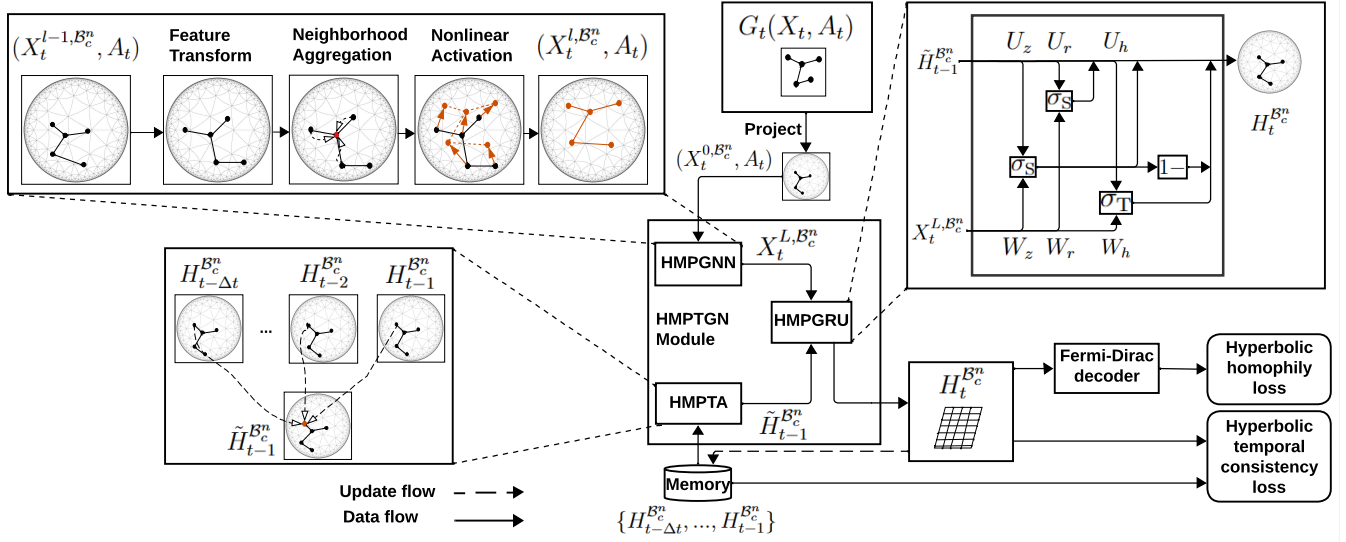


Figure 2: The overall architecture of our proposed HMPTGN, which includes the Hyperbolic Manifold-Preserving Graph Neural Network (HMPGNN), the Hyperbolic Manifold-Preserving Temporal Attention (HMPTA) and the Hyperbolic Manifold-Preserving Gated Recurrent Unit (HMPGRU). An additional Memory component is illustrated, which is used to store the previously learned representation for learning temporal relationship and training with the hyperbolic temporal consistency loss.

on normal matrix-vector multiplication. However, applying normal matrix-vector multiplication in hyperbolic space does not ensure that the transformed nodes reside on the manifold. To address this, we develop a *Poincaré linear transformation*, denoted by \otimes_c as follows:

$$y = W \otimes_c x = Wx, \text{ s.t. } W^T W = \mathbf{I}, \quad (10)$$

where x is a node embedded on the Poincaré ball \mathcal{B}_c^n , W is an orthogonal matrix, and \mathbf{I} is an identity matrix. The manifold-preserving property of the Poincaré linear transformation is proved in **Proposition 1**.

Proposition 1. *The Poincaré linear transformation ensures that the output node y lies on the Poincaré ball.*

Now, we can apply the Poincaré linear transformation to the node feature in hyperbolic space directly:

$$z_{t,i}^{l, \mathcal{B}_c^n} = W^l \otimes_c x_{t,i}^{l-1, \mathcal{B}_c^n} \oplus_c b^l, \quad (11)$$

where W^l , b^l are trainable parameters and $x_{t,i}^{l, \mathcal{B}_c^n}$ is the representation of node i at layer l on the manifold \mathcal{B}_c^n , i.e. $X_t^{l, \mathcal{B}_c^n} = \{x_{t,i}^{l, \mathcal{B}_c^n}\}_{i=1}^{|V|}$. For the bias addition \oplus_c with parameter b^l , the *Möbius addition* in Eq. (3) is employed. To learn the constrained parameter W^l effectively, we follow the work of [Lezcano-Casado, 2019].

Hyperbolic neighborhood aggregation. We utilize the Einstein midpoint [Ungar, 2005] in the Klein model as our aggregate function. Firstly, we map each node representation $z_{t,i}^{l, \mathcal{B}_c^n}$ obtained by the hyperbolic feature transformation in Eq. (11) to the Klein model via operation $p_{\mathcal{B}_c^n \rightarrow \mathcal{K}_c^n}$ in Eq. (5). Then we compute the aggregated representation of each

node i as the weighted Einstein midpoint:

$$z_{t,i}^{l, \mathcal{K}_c^n} = \frac{\sum_{j \in \mathcal{N}(i)} w_{ij} \gamma_j z_{t,j}^{l, \mathcal{K}_c^n}}{\sum_{j \in \mathcal{N}(i)} w_{ij} \gamma_j}, \quad (12)$$

where $\gamma_j = (1 - c \|z_{t,j}^{l, \mathcal{K}_c^n}\|^2)^{-1/2}$ is the Lorentz factor, $w_{ij} = ((\deg(j) + 1)(\deg(i) + 1))^{-1/2}$ is the normalized weight from GCN [Kipf and Welling, 2016a], $\deg(i)$ is the degree of node i , $\mathcal{N}(i)$ is the neighborhood of node i , $z_{t,j}^{l, \mathcal{K}_c^n}$ is the representation of node j in the Klein model. Finally, for each node i , the output $z_{t,i}^{l, \mathcal{K}_c^n}$ is projected back to the Poincaré ball by the reverse mapping $p_{\mathcal{K}_c^n \rightarrow \mathcal{B}_c^n}$ in Eq. (5). In comparison to H2H-GCN [Dai et al., 2021], our version includes an addition weight normalization trick to avoid exploding and vanishing gradient issues.

Hyperbolic nonlinear activation. The hyperbolic activation is given by:

$$x_{t,i}^{l, \mathcal{B}_c^n} = \sigma(z_{t,i}^{l, \mathcal{B}_c^n}). \quad (13)$$

The possible choices of σ include ReLU, Sigmoid, Tanh denoted as σ_R , σ_S , σ_T respectively. If we assume the input and output of the activation function are bounded, the following proposition guarantees that our HMPGNN is manifold-preserving on the Poincaré ball \mathcal{B}_c^n .

Proposition 2. *Given z such that $\|z\|^2 < \alpha$ and a nonlinear activation σ , such that $\|\sigma(z)\|^2 < \beta$, for known constants $\alpha, \beta > 0$. There exists a Poincaré ball \mathcal{B}_c^n that $z \in \mathcal{B}_c^n$ and $\sigma(z) \in \mathcal{B}_c^n$.*

Given the input and output of Eq. (13), it can be shown that all of the σ_R , σ_S , σ_T satisfy the manifold-preserving property. In practice, for training stability, one can increase the

radius value of the Poincaré ball \mathcal{B}_c^n to ensure the manifold-preserving property of σ .

By combining the feature transformation, neighborhood aggregation, and nonlinear activation, each layer of the HMPGNN module ensures that the output embedding stays on the Poincaré ball. After going through L layers of HMPGNN, we get the final node representation $X_t^{L, \mathcal{B}_c^n} = \{x_{t,i}^{L, \mathcal{B}_c^n}\}_{i=1}^{|V_t|}$ that contains the intact spatial structure information of the snapshot G_t in hyperbolic space.

4.2 Hyperbolic Manifold-Preserving Temporal Attention

To model the historical evolutionary information, we employ HMPTA, a temporal attention layer over a time window with fixed-length Δt . This approach is well-known for learning in dynamic graphs such as HGWaveNet [Bai *et al.*, 2023]. However, our proposed attention architecture is designed to work directly on the hyperbolic manifold instead of the tangent space, by using the Einstein midpoint.

Given a set of historical states of i^{th} node $\{h_{\tau,i}^{\mathcal{B}_c^n}\}_{\tau=t-\Delta t}^{t-1}$ as the input, the temporary historical state $\tilde{h}_{t-1,i}^{\mathcal{B}_c^n}$ is computed as follows. Firstly, we compute the attention coefficient μ_i across different historical states:

$$M_i = [h_{t-1,i}^{\mathcal{B}_c^n}, \dots, h_{t-\Delta t,i}^{\mathcal{B}_c^n}],$$

$$\mu_i = \text{softmax}(r^T \sigma_T(Q \otimes M_i)), \quad (14)$$

where the weight matrix Q and vector r are trainable, and \parallel is the concatenate operation. Then we apply the Einstein midpoint to achieve the final hidden state:

$$\tilde{h}_{t-1,i}^{\mathcal{K}_c^n} = \frac{\sum_{\tau=1.. \Delta t} \mu_{i,\tau} \gamma_\tau h_{t-\tau,i}^{\mathcal{K}_c^n}}{\sum_{\tau=1.. \Delta t} \mu_{i,\tau} \gamma_\tau}, \quad (15)$$

where $\gamma_\tau = (1 - c \|h_{t-\tau,i}^{\mathcal{K}_c^n}\|^2)^{-1/2}$ is the Lorentz factor, $h_{t-\tau,i}^{\mathcal{K}_c^n}$ is the corresponding embedding of the historical state $h_{t-\tau,i}^{\mathcal{B}_c^n}$ after projecting to the Klein model via $p_{\mathcal{B}_c^n \rightarrow \mathcal{K}_c^n}$ in Eq. (5). Lastly, we project the output $\tilde{h}_{t-1,i}^{\mathcal{K}_c^n}$ to the Poincaré ball via $p_{\mathcal{K}_c^n \rightarrow \mathcal{B}_c^n}$ in Eq. (5), to achieve the historical state $\tilde{h}_{t-1,i}^{\mathcal{B}_c^n}$.

The work of DHGAT [Li *et al.*, 2023] also utilizes the Einstein midpoint for temporal attention. However, DHGAT computes weights using hyperbolic distances between each pair of snapshots, resulting in a memory complexity of $O(|V_t| \Delta t^2 d)$, where d is representation dimension. In contrast, our HMPTA with the attention weights in (15) are computed on the linear memory M_i and has a memory complexity of $O(|V_t| \Delta t d)$.

4.3 Hyperbolic Manifold-Preserving Gated Recurrent Unit

By leveraging the Poincaré linear transformation in Eq. (13), we propose HMPGRU, a recurrent unit that works without tangent space, which is illustrated in Fig. 2. More formally, the HMPGRU module outputs the hidden representation $H_t^{\mathcal{B}_c^n}$ of the snapshot G_t using input pair $(X_t^{L, \mathcal{B}_c^n}, \tilde{H}_{t-1}^{\mathcal{B}_c^n})$, where X_t^{L, \mathcal{B}_c^n} represents the node features achieved from the

Algorithm 1 HMPTGN learning process

Input: List of snapshots $\{G_t(X_t, A_t)\}_{t=1}^{t=T}$
Output: List of hidden representations $\{H_t^{\mathcal{B}_c^n}\}_{t=1}^{t=T}$

- 1: Initialize memory $\Delta t \times \{H_0^{\mathcal{B}_c^n}\}$ and curvature c
- 2: **for** $t=1$ to T **do**
- 3: $X_t^{0, \mathcal{B}_c^n} = \exp_0^c(X_t)$
- 4: $X_t^{L, \mathcal{B}_c^n} = \text{HMPGNN}(X_t^{0, \mathcal{B}_c^n}, A_t)$
- 5: $\tilde{H}_{t-1}^{\mathcal{B}_c^n} = \text{HMPTA}(H_{t-1}^{\mathcal{B}_c^n}; \dots; H_{t-\Delta t}^{\mathcal{B}_c^n})$
- 6: $H_t^{\mathcal{B}_c^n} = \text{HMPGRU}(X_t^{L, \mathcal{B}_c^n}; \tilde{H}_{t-1}^{\mathcal{B}_c^n})$
- 7: $\mathcal{L}_t = \mathcal{L}_{t,c} + \lambda \mathcal{L}_{t,r}$
- 8: Minimize \mathcal{L}_t
- 9: Update memory
- 10: **end for**
- 11: **return** $\{H_t^{\mathcal{B}_c^n}\}_{t=1}^{t=T}$

HMPGNN module and $\tilde{H}_{t-1}^{\mathcal{B}_c^n}$ represents the temporary synthetic historical state from HMPTA module.

The *update gate* $P_t^{\mathcal{B}_c^n}$ and the *reset gate* $R_t^{\mathcal{B}_c^n}$ at timestamp t of HMPGRU, which balance the input and the memory, are computed as:

$$P_t^{\mathcal{B}_c^n} = \sigma_S((W_z \otimes_c X_t^{L, \mathcal{B}_c^n}) \oplus_c (U_z \otimes_c \tilde{H}_{t-1}^{\mathcal{B}_c^n})),$$

$$R_t^{\mathcal{B}_c^n} = \sigma_S((W_r \otimes_c X_t^{L, \mathcal{B}_c^n}) \oplus_c (U_r \otimes_c \tilde{H}_{t-1}^{\mathcal{B}_c^n})).$$

The current memory state $\tilde{H}_t^{\mathcal{B}_c^n}$ using the reset gate to store the relevant information from the past, is calculated as:

$$\tilde{H}_t^{\mathcal{B}_c^n} = \sigma_T((W_h \otimes_c X_t^{L, \mathcal{B}_c^n}) \oplus_c (U_h \otimes_c (R_t^{\mathcal{B}_c^n} \odot \tilde{H}_{t-1}^{\mathcal{B}_c^n}))).$$

The output latent representation $H_t^{\mathcal{B}_c^n}$ is then combined from the synthetic memory state and the current memory state:

$$H_t^{\mathcal{B}_c^n} = (1 - P_t^{\mathcal{B}_c^n}) \odot \tilde{H}_t^{\mathcal{B}_c^n} \oplus_c P_t^{\mathcal{B}_c^n} \odot \tilde{H}_{t-1}^{\mathcal{B}_c^n}, \quad (16)$$

where $W_z, W_r, W_h, U_z, U_r, U_h$ are the weight parameters, and \odot is the Hadamard product. Following the properties of the Sigmoid σ_S and Tanh σ_T functions in Proposition 2, all hidden representations $P_t^{\mathcal{B}_c^n}, R_t^{\mathcal{B}_c^n}$ reside on the Poincaré ball. Moreover, the manifold-preserving property of the Hadamard product is given by the following proposition:

Proposition 3. Given $x, p \in \mathcal{B}_c^n$ such that $0 \leq p_i \leq 1 \forall i = 1, \dots, n$. Then we have $x \odot p \in \mathcal{B}_c^n$.

Using this property of Hadamard product, it is straightforward to show that the output $H_t^{\mathcal{B}_c^n}$ in (16) stays on the Poincaré ball.

4.4 Overall Framework of HMPTGN

We summarize the HMPTGN learning process in Algorithm 1. Given a collection of snapshots $\{G_t(X_t, A_t)\}_{t=1}^{t=T}$ as the input, we want to extract contextual representations $\{H_t^{\mathcal{B}_c^n}\}_{t=1}^{t=T}$ which can be used to learn downstream tasks such as link prediction and new link prediction. Firstly, the memory states and the curvature of the Poincaré ball are initialized. The memory stores hidden representations of Δt snapshots before G_t . Let $\mathbf{0}$ be the origin point of the Poincaré ball

\mathcal{B}_c^n . For each snapshot G_t , the Euclidean node features X_t , which is assumed to be in $\mathcal{T}_0\mathcal{B}_c^n$, is mapped to the Poincaré ball \mathcal{B}_c^n via Eq. (7). Then the acquired node representation X_t^{0,\mathcal{B}_c^n} is sent to an L -layer HMPGNN unit. At the same time, multiple historical states from the memory $\{H_{\tau}^{\mathcal{B}_c^n}\}_{\tau=t-\Delta_t}^{\tau=t-1}$ are aggregated in HMPTA to achieve the temporary historical state $\tilde{H}_{t-1}^{\mathcal{B}_c^n}$. Finally, the outputs X_t^{L,\mathcal{B}_c^n} and $\tilde{H}_{t-1}^{\mathcal{B}_c^n}$ are given to HMPGRU to produce the hidden representation $H_t^{\mathcal{B}_c^n}$.

We employ the objective function \mathcal{L}_t in [Yang *et al.*, 2021] for training HMPTGN. The proposed \mathcal{L}_t is a weighted combination of the two losses: *Hyperbolic temporal consistency* $\mathcal{L}_{t,c}$ to ensure the temporal smoothness and long-term prediction ability; and *Hyperbolic homophily loss* $\mathcal{L}_{t,r}$ to maximize the probability of linked nodes through the hyperbolic features and minimize the probability of no interconnected nodes.

5 Experiments

5.1 Experiment Setup

Datasets. We evaluate our model and other baselines on 6 datasets: email communication networks Enron [Klimt and Yang, 2004]; academic co-author networks (COLAB) [Yang and Leskovec, 2012]; private messaging network system among students (UCI) [Panzarasa *et al.*, 2009]; synthetic dataset based on the SIR disease spreading model (Disease) [Bjørnstad *et al.*, 2002]; interactions network on the Math Overflow website (MO) [Paranjape *et al.*, 2016]; social network graph of Facebook Wall posts (FB) [Yang *et al.*, 2021].

Baselines. We compare the performance of HMPTGN with recent dynamic graph embedding methods in both Euclidean and hyperbolic space. Euclidean approaches include DySAT [Sankar *et al.*, 2018], EvolveGCN [Pareja *et al.*, 2019] VGRNN [Hajiramezanali *et al.*, 2020], and GRUGCN proposed in [Yang *et al.*, 2021], while hyperbolic approaches consist of HTGN [Yang *et al.*, 2021], HGWaveNet [Bai *et al.*, 2023] and DHGAT [Li *et al.*, 2023]. We also implement the HGRUHGCM model as a lightweight extension of GRUGCN by replacing GRU and GCN with Hyperbolic GRU and Hyperbolic GCN. Our implementation is available at the github repository <https://github.com/quanlv9211/HMPTGN>.

Evaluation Tasks and Metrics. Following HTGN [Yang *et al.*, 2021], we evaluate our HMPTGN on two downstream tasks: *temporal link prediction* and *temporal new link prediction*. In *temporal link prediction*, the model has to predict the edges that appear in $\{G_{t+1}, G_{t+2}, \dots\}$ after being trained on $\{G_1, G_2, \dots, G_t\}$. Meanwhile, *temporal new link prediction* aims to predict edges in G_τ but not in $G_{\tau-1}$ for any snapshot index $\tau > t$. The reported metrics care about average precision (AP) and area under the ROC curve (AUC). We choose the last k snapshots as the test set and the rest as the training set. To ensure a balanced measurement, we consider all edges within the test set as true and randomly sample an equivalent number of unconnected edges as false.

5.2 Experimental Results

We run the experiments with three different seeds and report the average value with standard deviation on the test sets in Table 1 and 2. The best results are in **bold** and the second-best results are in underline for each dataset.

Temporal link prediction. It can be clearly seen that our proposed model outperforms the competing methods on most datasets on both learning tasks, including non-hyperbolic and hyperbolic approaches. Only the recent HGWaveNet has slightly better results than the HMPTGN in the UCI dataset, while the former achieves lower performances on the remaining datasets. On very large graphs (e.g. MO, FB), DHGAT suffers from the out-of-memory (OOM) problem because of the memory complexity in its temporal attention function. Meanwhile, our HMPTGN achieves average gains of 1.92% in AUC and 1.93% in AP compared to the best baseline.

Temporal new link prediction The results on temporal new link prediction are shown in Table 2. Note that the new link prediction task is more challenging since it requires the model to classify a link that only appears in future snapshots. Our model consistently outperforms the other baselines on most datasets. Moreover, in the Disease benchmark, our model has a significant improvement, gaining 10.32% in AUC and 13.48% in AP compared to the second-best baseline. One of the main reasons is the Disease dataset has a well-defined hierarchical structure. Besides, it has many unseen nodes and edges in the test set, which makes the distortion error more critical to the hyperbolic-based representation.

5.3 Ablation Study

We additionally perform an ablation study to highlight the superiority of the manifold-preserving property in the main components of HMPTGN. Firstly, we create three variants of HMPTGN, which are **w/o HMPGNN**, **w/o HMPTA**, and **w/o HMPGRU**. The three variants are created by removing the manifold-preserving property in that specific component and relying on tangent space to learn the embedding. Then, we evaluate these variants on the Disease dataset with three different seeds. The results are reported in Table 3. In general, removing manifold-preserving property in any component would lower the model’s performance. **w/o HMPGNN** leads to a decline in the model’s performance by 2% in average. This is because tangent space has distorted the spatial structure of the graph. Meanwhile, changing to **w/o HMPTA** leads to a significant decrease in the link prediction task. This suggests that the temporal information carried in the previous snapshots is more accurately obtained on the original manifold compared to the tangent space. Similarly, in the case of **w/o HMPGRU**, the model’s performance also drops dramatically in both tasks. The results affirm the superiority of our hyperbolic preserving modules in comparison to their tangent-based counterparts.

6 Related Works

Dynamic Graph Embedding. There exist diverse techniques for embedding dynamic graphs such as matrix factorization methods [Rossi *et al.*, 2013] or random walk methods

Datasets	Disease		Enron		COLAB		UCI		MO		FB	
Metric	AUC \uparrow	AP \uparrow	AUC \uparrow	AP \uparrow	AUC \uparrow	AP \uparrow	AUC \uparrow	AP \uparrow	AUC \uparrow	AP \uparrow	AUC \uparrow	AP \uparrow
DySAT	78.46 \pm 3.21	72.58 \pm 1.68	89.28 \pm 0.76	88.62 \pm 1.19	79.83 \pm 0.80	79.08 \pm 2.00	75.74 \pm 5.35	82.63 \pm 2.75	83.23 \pm 2.17	84.31 \pm 1.90	67.49 \pm 0.21	71.02 \pm 0.05
EvolveGCN	69.25 \pm 1.43	67.59 \pm 1.20	90.43 \pm 0.45	92.85 \pm 0.22	83.16 \pm 0.34	87.42 \pm 0.35	85.10 \pm 2.40	88.08 \pm 1.07	69.60 \pm 2.47	75.19 \pm 0.06	75.59 \pm 0.13	79.97 \pm 0.16
VGRNN	83.69 \pm 0.78	79.58 \pm 1.76	87.89 \pm 0.29	86.95 \pm 0.17	77.45 \pm 0.52	79.11 \pm 0.48	79.76 \pm 0.92	82.68 \pm 0.73	OOM		OOM	
GRUGCN	87.43 \pm 1.71	86.51 \pm 1.70	92.16 \pm 0.21	92.82 \pm 0.23	83.66 \pm 0.19	86.27 \pm 0.35	73.86 \pm 1.01	81.37 \pm 0.45	67.70 \pm 3.24	77.56 \pm 2.13	78.25 \pm 0.56	81.36 \pm 0.38
HGRUHCN	80.56 \pm 0.38	78.89 \pm 0.62	91.55 \pm 1.42	92.14 \pm 1.26	83.10 \pm 0.73	87.03 \pm 0.37	80.97 \pm 0.83	83.19 \pm 1.19	59.06 \pm 0.32	71.26 \pm 0.47	75.72 \pm 0.25	76.95 \pm 0.39
HTGN	82.66 \pm 1.04	75.45 \pm 1.94	93.38 \pm 0.26	93.73 \pm 0.23	87.78 \pm 0.52	90.17 \pm 0.31	90.55 \pm 0.11	90.02 \pm 0.34	86.08 \pm 0.05	85.30 \pm 0.16	82.29 \pm 0.09	78.38 \pm 0.79
HGWaveNet	83.80 \pm 0.43	73.59 \pm 2.46	94.33 \pm 0.17	94.39 \pm 0.14	88.23 \pm 0.19	90.52 \pm 0.22	91.86 \pm 0.16	91.92 \pm 0.15	85.70 \pm 0.46	85.15 \pm 0.55	82.12 \pm 0.82	78.06 \pm 1.60
DHGAT	91.23 \pm 0.22	89.44 \pm 0.40	94.27 \pm 0.24	93.82 \pm 0.40	89.13 \pm 0.80	90.98 \pm 0.47	79.14 \pm 0.35	81.92 \pm 0.30	OOM		OOM	
HMPTGN(ours)	91.45 \pm 0.42	88.23 \pm 0.79	95.09 \pm 0.27	95.17 \pm 0.21	89.51 \pm 0.11	91.54 \pm 0.04	<u>91.52 \pm 0.48</u>	<u>91.89 \pm 0.51</u>	86.53 \pm 0.46	86.34 \pm 0.29	85.02 \pm 0.27	83.50 \pm 0.14
Gain(%)	+ 0.24	- 1.37	+ 0.81	+ 0.83	+ 0.43	+ 0.62	- 0.37	- 0.03	+ 0.52	+ 1.22	+ 3.32	+ 2.63

 Table 1: The results of our model and other baselines on *temporal link prediction* task.

Datasets	Disease		Enron		COLAB		UCI		MO		FB	
Metric	AUC \uparrow	AP \uparrow	AUC \uparrow	AP \uparrow	AUC \uparrow	AP \uparrow	AUC \uparrow	AP \uparrow	AUC \uparrow	AP \uparrow	AUC \uparrow	AP \uparrow
DySAT	75.67 \pm 1.78	64.49 \pm 0.53	83.19 \pm 0.22	82.16 \pm 0.65	71.27 \pm 0.54	70.23 \pm 1.69	71.50 \pm 5.18	78.68 \pm 3.09	82.98 \pm 2.23	84.74 \pm 1.93	65.89 \pm 0.10	69.34 \pm 0.27
EvolveGCN	59.05 \pm 0.73	53.62 \pm 0.91	83.92 \pm 0.21	86.11 \pm 0.08	72.09 \pm 0.64	76.87 \pm 0.65	81.91 \pm 2.42	85.18 \pm 0.87	71.58 \pm 2.38	77.01 \pm 0.17	73.14 \pm 0.15	77.33 \pm 0.18
VGRNN	82.11 \pm 7.34	73.75 \pm 9.29	80.99 \pm 1.03	78.53 \pm 0.33	67.85 \pm 0.78	69.78 \pm 0.42	75.61 \pm 1.74	78.72 \pm 1.32	OOM		OOM	
GRUGCN	61.80 \pm 4.22	52.15 \pm 2.60	85.80 \pm 0.23	86.31 \pm 0.33	75.43 \pm 0.88	77.74 \pm 1.06	70.00 \pm 1.04	78.48 \pm 0.57	69.97 \pm 2.76	79.31 \pm 1.83	76.69 \pm 0.58	79.79 \pm 0.39
HGRUHCN	76.51 \pm 6.31	64.48 \pm 5.59	85.53 \pm 2.03	85.67 \pm 1.45	74.41 \pm 1.39	78.32 \pm 0.80	77.91 \pm 0.31	80.04 \pm 0.29	63.29 \pm 0.24	74.21 \pm 0.34	74.23 \pm 0.37	75.27 \pm 0.31
HTGN	77.54 \pm 0.86	69.50 \pm 5.04	88.51 \pm 0.47	87.62 \pm 0.50	79.98 \pm 0.99	81.89 \pm 0.56	88.98 \pm 0.34	88.24 \pm 0.45	85.78 \pm 0.07	85.56 \pm 0.10	81.03 \pm 0.02	77.08 \pm 0.70
HGWaveNet	76.34 \pm 4.21	62.99 \pm 4.01	89.69 \pm 0.15	88.60 \pm 0.36	80.52 \pm 0.38	82.19 \pm 0.55	90.06 \pm 0.54	89.96 \pm 0.40	85.53 \pm 0.40	85.45 \pm 0.60	80.82 \pm 0.84	76.68 \pm 1.54
DHGAT	79.65 \pm 0.63	68.46 \pm 0.84	<u>90.01 \pm 0.21</u>	87.01 \pm 0.58	<u>81.52 \pm 1.06</u>	82.01 \pm 0.54	76.60 \pm 0.31	78.85 \pm 0.48	OOM		OOM	
HMPTGN(ours)	90.58 \pm 0.79	83.69 \pm 0.72	90.72 \pm 0.50	89.23 \pm 0.05	82.29 \pm 0.40	84.06 \pm 0.21	<u>89.23 \pm 0.18</u>	<u>89.36 \pm 0.19</u>	86.04 \pm 0.40	86.39 \pm 0.20	83.74 \pm 0.39	81.75 \pm 0.19
Gain(%)	+ 10.32	+ 13.48	+ 0.56	+ 0.71	+ 0.94	+ 2.76	- 0.93	- 0.67	+ 0.30	+ 0.97	+ 3.34	+ 2.46

 Table 2: The results of our model and other baselines on *temporal new link prediction* task.

Task	Link prediction		New link prediction	
Metric	AUC \uparrow	AP \uparrow	AUC \uparrow	AP \uparrow
HMPTGN	91.45 \pm 0.42	88.23 \pm 0.79	90.58 \pm 0.79	83.69 \pm 0.72
w/o HMPGNN	88.81 \pm 0.85	85.12 \pm 1.20	88.54 \pm 0.50	81.16 \pm 0.91
Gain(%)	- 2.89	- 3.52	- 2.25	- 3.02
w/o HMPTA	83.78 \pm 1.08	77.57 \pm 1.74	86.21 \pm 0.94	81.45 \pm 0.70
Gain(%)	- 8.39	- 12.08	- 4.82	- 2.68
w/o HMPGRU	84.48 \pm 1.58	80.53 \pm 1.82	76.00 \pm 1.76	71.15 \pm 1.80
Gain(%)	- 7.62	- 8.73	- 16.10	- 14.98

Table 3: Ablation study on the effect of manifold-preserving property in each main module of HMPTGN on the Disease dataset.

[Nguyen *et al.*, 2018]. Recently, deep learning approaches employ neural networks to extract the topological properties and capture temporal dependencies of dynamic graphs, leading to state-of-the-art performances. For instance, DySAT [Sankar *et al.*, 2018] creates node representation through joint self-attention along the spatial and temporal dimensions. VRGNN [Hajiramezanali *et al.*, 2020] enhances the expressive capability by inputting the node embedding generated by VGAE [Kipf and Welling, 2016b] on each snapshot into the hidden state of a graph recurrent network. EvolveGCN [Pareja *et al.*, 2019] incorporates an RNN to update the parameters of the GCNs [Kipf and Welling, 2016a].

Hyperbolic Graph Embedding. Hyperbolic geometry has been utilized in the static graph domain due to its efficiency for modeling data with latent hierarchies [Chen *et al.*, 2021a; Peng *et al.*, 2021; Chen *et al.*, 2021b; Yang *et al.*, 2023]. Recent works [Liu *et al.*, 2019; Chami *et al.*, 2019] extend graph convolution to hyperbolic space by shifting the aggregate operation to the tangent space, enabling the execution of vector operations and leading to the superior performance. However, it is important to note that a tangent space serves as a first-order approximation of the original space and can potentially cause distortion. [Dai *et al.*, 2021] propose H2H-GCN

working directly on the hyperbolic manifold to keep the geometric structure of the graph. In hyperbolic dynamic graph learning, [Yang *et al.*, 2021] propose HTGN, incorporating hyperbolic GNN and hyperbolic GRU to capture spatial and temporal dependencies in dynamic graphs. HGWaveNet [Bai *et al.*, 2023] employs hyperbolic diffusion graph convolution to obtain the structural information of nodes and uses hyperbolic dilated causality convolution to acquire causal relationships between snapshots. DHGAT [Li *et al.*, 2023] employs a hyperbolic self-attention that operates directly on the manifold. However, DHGAT still relies on the tangent space to conduct feature transformation and nonlinear activation.

7 Conclusion

In this paper, we first analyze the drawbacks of tangent space in hyperbolic dynamic graph learning. The tangent space can weaken the learning capabilities of traditional hyperbolic methods. Therefore, we propose HMPTGN, a hyperbolic dynamic graph method that can work directly on the Poincaré manifold. The HMPTGN consists of three main components to model spatial and temporal relationships in the dynamic graph. Experiment results on real-world datasets demonstrate that our model surpasses the Euclidean-based and other hyperbolic-based methods. Overall, our proposed approach highlights the efficiency of applying hyperbolic space to model the complexity of discrete-time dynamic graphs. The results can also be extended to incorporate different hyperbolic models beyond the Poincaré ball for modeling the dynamic graph embedding.

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