Hyperbolic Variational Graph Neural Network for Modeling Dynamic Graphs

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Abstract

Learning representations for graphs plays a critical role in a wide spectrum of downstream applications. In this paper, we summarize the limitations of the prior works in three folds: representation space, modeling dynamics and modeling uncertainty. To bridge this gap, we propose to learn dynamic graph representation in hyperbolic space, for the first time, which aims to infer stochastic node representations. Working with hyperbolic space, we present a novel Hyperbolic Variational Graph Neural Network, referred to as HVGNN. In particular, to model the dynamics, we introduce a Temporal GNN (TGNN) based on a theoretically grounded time encoding approach. To model the uncertainty, we devise a hyperbolic graph variational autoencoder built upon the proposed TGNN to generate stochastic node representations of hyperbolic normal distributions. Furthermore, we introduce a reparameterisable sampling algorithm for the hyperbolic normal distribution to enable the gradient-based learning of HVGNN. Extensive experiments show that HVGNN outperforms state-of-the-art baselines on real-world datasets.

Introduction

Recent years have witnessed a surge of representation learning on graphs (Perozzi, Al-Rfou, and Skiena 2014; Tang et al. 2015; Xhonneux, Qu, and Tang 2020). Its basic idea is to map each node to a vector in a low-dimensional representation space. By learning graph representations, classical machine learning algorithms (Xia et al. 2020) can be applied to solve various graph analysis tasks, such as link prediction and node classification (Kipf and Welling 2016a).

In this paper, we summarize the limitations of the prior graph representation learning works in three folds:

1) **Representation Space.** Most of existing studies (Kipf and Welling 2016b; Xu et al. 2020) model graphs in the Euclidean space. Euclidean models tend to have distortions when representing real-world graphs with latent hierarchies (Chami et al. 2019; Chen et al. 2013). In particular, for such graphs, the number of nodes surrounding to a center node grows exponentially w.r.t. radius. However, the size of the Euclidean space only grows polynomially w.r.t. radius, while this size grows exponentially in hyperbolic space (Krioukov et al. 2010). **Hyperbolic space** provides a more promising alternative. Actually, recent results (Papadopoulos et al. 2012; Liu, Nickel, and Kiela 2019) show that hyperbolic space is well-suited for modeling graphs.

2) **Modeling Dynamics.** Most of existing models (Li et al. 2020; Tu et al. 2018; Wang, Cui, and Zhu 2016) consider the graphs to be static. Actually, graphs are usually dynamic and constantly evolving over time. Dynamic graphs have been typically observed in social networks, transportation networks and financial transaction networks (Zhou et al. 2018b). Ignoring the inherent dynamics of graphs usually leads to questionable inference. Such models may mistakenly utilize future information for predicting past interactions as the evolving constraints are disregarded.

3) **Modeling Uncertainty.** Most of existing models (Liu et al. 2020; Grover and Leskovec 2016) map nodes to deterministic vectors. However, the formation and evolution of graphs are full of uncertainties, especially for low-degree nodes which deliver less information and bear more uncertainties (Zhu et al. 2018). Actually, uncertainty is an inherent characteristic of graphs. The deterministic representation cannot model uncertainty. Alternatively, **stochastic** representation provides a promising approach to model such characteristic. It naturally captures the uncertainty to represent nodes as normal distributions, i.e., the mean and variance.

To address the aforementioned limitations, we propose to learn dynamic graph representation in hyperbolic space, for the first time, which aims to learn stochastic node representations modeling graph dynamics and its uncertainty.

To this end, we present a novel Hyperbolic Variational Graph Neural Network, referred to as HVGNN. In HVGNN, to address the first limitation, instead of the Euclidean space, we utilize hyperbolic space as the representation space. To address the second limitation, we introduce a novel Temporal GNN (TGNN) to model the dynamics. In particular, TGNN performs a time-aware attention based on a theoretically grounded time encoding approach, which distinguishes nodes in time domain. To address the third limitation, we devise a hyperbolic graph variational autoencoder built upon TGNN to jointly model the uncertainty and dy-
namics. In particular, we generate stochastic representations of wrapped normal distributions, the generalized normal distributions in hyperbolic space, whose parameters are defined by TGNN. Furthermore, we introduce a reparameterisable sampling algorithm for wrapped normal distributions to enable the gradient-based learning of HVGNN.

We evaluate HVGNN by two typical downstream tasks on graph data: link prediction and node classification. Extensive experiments on real-world datasets show that HVGNN outperforms several state-of-the-art methods.

Overall, main contributions of our work are listed below:

- To the best of our knowledge, this is the first attempt to learn the node representations for dynamic graphs in hyperbolic space.
- We propose a novel Hyperbolic Variational Graph Neural Network, HVGNN, which generates stochastic representations to model graph dynamics and its uncertainty in hyperbolic space.
- Experimental results show the superiority of HVGNN on several real-world datasets.

Preliminaries: Hyperbolic Geometry

Prior to introducing the studied problem and proposed approach, we provide some important preliminaries about hyperbolic geometry in this section. For in-depth expositions, refer mathematical materials (Loomis 2013; Hopper and Andrews 2010). Throughout the paper, we denote the Euclidean norm and inner product by $|| \cdot ||$ and $(\cdot , \cdot )$, respectively.

Riemannian Manifold

A manifold $M$ is a space that generalizes the notion of a 2D surface to higher dimensions (Ganea, Bécigneul, and Hofmann 2018). For each point $x \in M$, it associates with a tangent space $T_xM$ of the same dimensionality as $M$. Intuitively, $T_xM$ contains all possible directions in which one can pass through $x$ tangentially. On the associated tangent space $T_xM$, the Riemannian metric, $g_x(\cdot , \cdot ) : T_xM \times T_xM \to \mathbb{R}$, defines an inner product specifying the geometry of $M$. A Riemannian manifold is then defined as the tuple of $(M, g)$.

Mapping between the tangent space and the manifold is done via exponential and logarithmic maps. For a point $x \in M$ in the manifold, the exponential map at $x$, $\exp_x(v) : T_xM \to M$, projects the vector $v \in T_xM$ onto the manifold $M$. The logarithmic map at $x$, $\log_x(y) : M \to T_xM$, projects the vector $y \in M$ back to the tangent space $T_xM$. Mapping between tangent spaces is done via parallel transport. For two points $x, y \in M$ in the manifold, the parallel transport from $x$ to $y$, $P_{x \to y}(v) : T_xM \to T_yM$, carries the vector $v \in T_xM$ to $T_yM$ along the geodesic, a smooth path on the manifold of minimal length between $x$ and $y$.

As one of the fundamental objects, the hyperbolic space is a Riemannian manifold with constant negative curvature. There are four common equivalent models of hyperbolic space: the Poincaré disk model, Poincaré half-plane model, Lorentz (aka hyperboloid/Minkowski) model and Klein model (Liu, Nickel, and Kiela 2019). Next, we give more details of the latter two, which will both be utilized in this paper, for further discussions.

The Lorentz Model

We denote $L^{d,K}$ as the Lorentz model in $d$ dimensions with constant negative curvature $-1/K$ where $K > 0$. The Lorentz model $L^{d,K}$ is defined on a subset of $\mathbb{R}^{d+1}$, $L^{d,K} = \{ x \in \mathbb{R}^{d+1} | (x, x)_L = -K \}$, where $(\cdot , \cdot )_L : \mathbb{R}^{d+1} \times \mathbb{R}^{d+1} \to \mathbb{R}$ is Lorentzian inner product defined as,

$$(x, y)_L = -x_0y_0 + x_1 y_1 + x_2 y_2 + \cdots + x_d y_d.$$ (1)

We denote $\mathbb{T}_x L^{d,K}$ as the tangent space of $x \in L^{d,K}$. We have $\mathbb{T}_x L^{d,K} = \{ v \in \mathbb{R}^{d+1} | (v, x)_L = 0 \}$ and $||v||_L = \sqrt{(v, v)_L}$ is the norm of $v$. For $u, v \in \mathbb{T}_x L^{d,K}$, we can give the Riemannian metric tensor $g^L_{x}(u, v) = (v, u)_L$. Next, we give the closed form equations of exponential map, logarithmic map and parallel transport. For any $x, y \in L^{d,K}$ and $v \in \mathbb{T}_x L^{d,K}$, we have the following equations:

$$\exp^L(v) = \cosh \left( \frac{||v||_L}{\sqrt{K}} \right) x + \sqrt{K} \sinh \left( \frac{||v||_L}{\sqrt{K}} \right) \frac{v}{||v||_L},$$ (2)

$$\log^L(y) = \frac{d^L_2(x, y)}{y + \sqrt{K} (x, y)_L x} / \sqrt{K}(x, y)_L x,$$ (3)

$$P^L_{x \to y}(v) = v - \log^L(\exp^L(v, y)_L),$$ (4)

where $d^L_2(x, y) = \sqrt{K} \cosh^{-1}(-/(x, y)_L/K)$. The Klein Model

We denote $\mathbb{K}^{d,K}$ as the Klein model in $d$ dimensions with constant negative curvature $-1/K$ where $K > 0$. The Klein model $\mathbb{K}^{d,K}$ is defined on a subset of $\mathbb{R}^d$, $\mathbb{K}^{d,K} = \{ x \in \mathbb{R}^d | \|x\|^2 < K \}$. A point $x \in \mathbb{K}^{d,K}$ is projected from the corresponding $y \in L^{d,K}$. We derive the projection with the $i$th entry:

$$\pi^K_{\mathbb{R} \to \mathbb{K}}(y_i) = \sqrt{K} \frac{y_i}{y_0},$$ (5)

whose inverse is given as

$$\pi^K_{\mathbb{K} \to \mathbb{R}}(x) = \eta^K(x)(\sqrt{K} x), \eta^K(x) = \sqrt{\frac{K}{K - \|x\|^2}},$$ (6)

where $\eta^K(x)$ is the function defining the Lorentz factor, and $(\cdot , \cdot)$ denotes concatenation.

Problem Definition

In this paper, we consider a dynamic graph where edges evolve over time. The emergence/disappearance of nodes will lead to the addition/deletion of a set of incident edges concurrently, which can be easily modeled with our proposed approach in a similar way. Formally, we give the definition of a dynamic graph as follows:

Definition 1 (Dynamic Graph). A dynamic graph is defined as a triple $G = (V, E, T)$, where $V = \{v_1, v_2, \cdots, v_n\}$ is the node set and each node $v_i$ is associated with a feature vector $x_i \in \mathbb{R}^f$. $E = \{ (v_i, v_j) \}$ is the edge set, and $T = \{ t_k \}$ is the timestamp set. Each edge $(v_i, v_j)$ is associated with a timestamp $t_k \in T$ representing that $v_i$ and $v_j$ interact with each other at time $t_k$.

Without loss of generality, we consider the dynamic graph to be attributed. The timestamps on edges record every interaction among nodes, and thereby fine-grained graph dy-
Riemannian metric of hyperbolic space, in the patterns between the relative timespan. Thus, in learning the map, it is of paramount importance to identify a function \( \psi : [-t_{\text{max}}, t_{\text{max}}] \to \mathbb{R} \) that reveals critical temporal information.

We utilize this approach for hyperbolic modeling of dynamics. Formally, we aim to learn a map \( \psi : \mathbb{H}^d \to \mathbb{H}^d \) that, for each node \( v_i \), we can infer a stochastic representation \( \mathbf{z}_i(t) \) at any time \( t \) in hyperbolic space \( \mathbb{H}^d \).

The stochastic representation is drawn from a generalized normal distribution in hyperbolic space, modeling graph dynamics and its uncertainty.

**HVGNN: Hyperbolic Variational GNN**

In this section, we present a novel Hyperbolic Variational Graph Neural Network (HVGNN) for dynamic graph representations in hyperbolic space. In a nutshell, HVGNN generates stochastic representations jointly modeling graph dynamics and uncertainty. Specifically, to model the dynamics, we propose a novel Temporal Graph Neural Network (TGNN). To model the uncertainty, we introduce a hyperbolic Variational Graph AutoEncoder (VGAE), where we utilize TGNNN as encoder and give task-oriented decoder for specific tasks, e.g., link prediction and node classification. Next, we elaborate on the building blocks of HVGNN, i.e., temporal GNN and hyperbolic VGAE, respectively.

**Temporal GNN**

We propose the novel TGNNN to model graph dynamics in two types of representation spaces: hyperbolic space \( \mathbb{H}^d \) and Euclidean space \( \mathbb{E}^d \). Similar to GAT (Veličković et al., 2018), the basic idea of TGNNN follows the graph attention network. However, the attention itself cannot handle graph dynamics. To bridge this gap, the key is to design the following theoretically grounded time encoding approach, distinguishing nodes in time domain.

**Hyperbolic Time Encoding**

We propose a novel time encoding approach to equip graph attention with the ability of modeling dynamics. Formally, we aim to learn a map \( \phi : T \to \mathbb{H}^d \) from a point in time domain \( T \) to a vector in hyperbolic space \( \mathbb{H}^d \), encoding the temporal dependencies. The time domain \( T \) is defined as \([0, t_{\text{max}}]\) and \( t_{\text{max}} \) denotes the maximum time point in the observed data.

Usually, it is the relative timespan rather than the absolute value of time that reveals critical temporal information. Thus, in learning the map \( \phi : T \to \mathbb{H}^d \), we are interested in the patterns between the relative timespan \([t_i - t_j]\) and the Riemannian metric of hyperbolic space, i.e., Lorentzian inner product. We thereby define a Lorentzian kernel \( K_{\phi} : T \times T \to \mathbb{H}^d \) with \( K_{\phi}(t_i, t_j) = \langle \phi(t_i), \phi(t_j) \rangle \). It is ideal that the kernel can be expressed as a function of relative timespan, namely, translation invariance. Formally, \( K_{\phi}(t_i, t_j) = \psi(\mathbf{t}_j - \mathbf{t}_i) \) for some function \( \psi : [-t_{\text{max}}, t_{\text{max}}] \to \mathbb{R} \).

Instead of investigating \( K_{\phi}(t_i, t_j) \) explicitly, we propose a two-step approach for hyperbolic time encoding as follows:

**Step 1:** Construct a translation invariant Euclidean time encoding map. We study its Euclidean counterpart \( K_{\psi}(t_i, t_j) = \langle \phi_{\psi}(t_i), \phi_{\psi}(t_j) \rangle \) where \( \phi_{\psi} : T \to \mathbb{R}^d \). Note that \( K_{\psi} \) is positive semidefinite as it is defined by Euclidean inner product. Accordingly, we have \( K_{\psi} \) translation invariant, \( K_{\psi}(t_i, t_j) = \psi(t_i - t_j) \). Thus, \( K_{\psi} \) satisfies the assumption of the Bochner’s theorem (Loomis 2013): A translation-invariant kernel \( K_{\psi}(t_i, t_j) = \psi(t_i - t_j) \) is positive definite iff there exists a nonnegative measure \( \rho(\omega) \) on \( \mathbb{R}^d \) such that \( \psi(\mathbf{t}) = \mathbb{F}[\rho(\omega)] \).

According to the Bochner’s theorem, we have

\[
K_{\psi}(t_i, t_j) = \int_{\mathbb{R}^d} e^{i \omega(t_i - t_j)} \rho(\omega) d\omega = \mathbb{E}_\omega \left[ \mathbb{E}_\omega \left( \xi_i(t_i) \xi_j(t_j) \right) \right],
\]

where \( \xi_i(t_i) = e^{i \omega t_i}, i \) is the imaginary unit, and \( \mathbb{E} \) denotes the conjugate complex. As both kernel \( K_{\psi} \) and its associated map \( \phi_{\psi} \) are real, we extract the real part of the expectation in Eq. (7), which can be approximated by Monte Carlo integral (Rahimi and Recht 2007), i.e.,

\[
K_{\psi}(t_i, t_j) = \frac{1}{n} \sum_{i=1}^{n} \cos(\omega_i t_i) \cos(\omega_i t_j) + \sin(\omega_i t_i) \sin(\omega_i t_j).
\]

According to the formulation above, we define \( \phi_{\psi} \) below,

\[
\phi_{\psi}(t) = \sqrt{\frac{n}{2}} \cos(\omega t + \theta_1) + \cos(\omega t + \theta_2) + \cdots + \cos(\omega d + \theta_d),
\]

where \((\cdot, \cdot)\) denotes the concatenation, and we will learn the \( \omega \)s and \( \theta \)s with different subscripts as model parameters.

**Step 2:** Project Euclidean time encoding to the hyperbolic space. We refer to \((\sqrt{K}, 0, \cdots, 0)\) as the origin of Lorentzian model, denoted as \( \mathbb{O} \). For \( x \in \mathbb{R}^d \), we have \((0, x) \) live in the tangent space of the origin \( T_{\mathbb{O}} \mathbb{H}^d \), since \( T_{\mathbb{O}} (0, x) \otimes_\mathbb{O} = 0 \). Then, \((0, x) \) can be projected onto \( \mathbb{H}^d \) via the exponential map. Finally, we define the projection as

\[
\pi_{\mathbb{O}}^K(x) = \exp_{\mathbb{O}}^K((0, x)),
\]

and obtain \( \phi_e(t) = \pi_{\mathbb{O}}^{-K}(\phi_{\psi}(t)), i.e., \phi_e(t) = (\sqrt{K} \cosh(\sqrt{\frac{n}{2}} \| \phi_{\psi}(t) \|) - \sqrt{\frac{n}{2}} \| \phi_{\psi}(t) \|) \phi_{\psi}(t).
\]

Now, we prove the translation invariance of Lorentzian kernel \( K_{\phi}(t_i, t_j) \) with the hyperbolic time encoding map \( \phi_e \).

**Theorem 1 (Translation Invariance)**

The Lorentzian kernel \( K_{\phi_e}(t_i, t_j) = \langle \phi_{\phi_e}(t_i), \phi_{\phi_e}(t_j) \rangle \) with the proposed \( \phi_e(t) \) is translation invariant, i.e., \( K_{\phi_e}(t_i, t_j) = \psi_e(t_i - t_j) \).

**Proof.**

We prove the translation invariance of the Lorentzian kernel \( K_{\phi_e}(t_i, t_j) \) by proving the existence of the function \( \psi_e \). Expanding the Lorentzian product with the definition given in Eq. (1), we have the following equation hold,

\[
\langle \phi_{\phi_e}(t_i), \phi_{\phi_e}(t_j) \rangle = A(\phi_{\psi}(t_i), \phi_{\psi}(t_j)) + B,
\]

where

\[
A = -K \sinh(\frac{\phi_{\psi}(t_i)}{\sqrt{R}}) \sinh(\frac{\phi_{\psi}(t_j)}{\sqrt{R}}) \frac{1}{\| \phi_{\psi}(t_i) \| \| \phi_{\psi}(t_j) \|},
\]

\[
B = -K \cosh(\frac{\phi_{\psi}(t_i)}{\sqrt{R}}) \cosh(\frac{\phi_{\psi}(t_j)}{\sqrt{R}}) \frac{1}{\| \phi_{\psi}(t_i) \| \| \phi_{\psi}(t_j) \|},
\]

(13)
According to the Bochner’s theorem, we have $K(t_i, t_j) = \langle \phi_E(t_i), \phi_E(t_j) \rangle = \psi_E(t_i - t_j)$. Thus, for given $t_i$ and $t_j$, $K(t_i, t_j) = \langle \phi_E(t_i), \phi_E(t_j) \rangle = \psi_E(t_i - t_j)$, where $\psi^2 = f \circ \psi^R$ and $f(x) = Ax + B$. Refer Supplementary Material for further details.

**Hyperbolic Operators** We introduce the hyperbolic operators required by hyperbolic TGN. In particular, we generalize aggregation, addition and linear transformation from Euclidean space $\mathbb{R}^d$ to hyperbolic space $\mathbb{L}^{d,K}$. Aggregation is to calculate a weighted midpoint in Euclidean space (Gulcehre et al. 2019). The Euclidean midpoint is generalized to Einstein midpoint in hyperbolic space. Specifically, we have a vector set $\{x_i | x_i \in \mathbb{L}^{d,K}, i \in \Omega\}$, where $\Omega$ is the index set and each $x_i$ is associated with a weight $a_i$. Their Einstein midpoint $\text{AGG}^K(\{a_i, x_i | i \in \Omega\})$ is calculated as

$$\text{AGG}^K(\{a_i, x_i | i \in \Omega\}) = \sum_i \frac{a_i \psi^K(x_i)}{\sum_j a_j \psi^K(x_j)} x_i,$$

where $\psi^K(\cdot)$ is defined in Eq. (6), and $x$’s are the coordinates in Klein model. Fortunately, different models of hyperbolic space are essentially the same. We can transform coordinates between Klein and Lorentz model via Eqs. (5) and (6). Additionally, we regard the weighted addition $\oplus^K$ as its special, and have $x_1 \oplus^K x_2 = \text{AGG}^K(\{a_1, x_1 | a_2, x_2 | i \in \{1,2\}\})$.

Linear transformation in hyperbolic space is realized by matrix vector multiplication, denoted as $\otimes^K$. We define $\otimes^K$ via exponential and logarithmic maps as follows:

$$W \otimes^K x = \exp^K_D(W \log^K_D(x)),$$

where $W$ is the weight matrix. The intuition is that we perform linear transformation in the Euclidean tangent space and then map the result back onto hyperbolic space.

**Hyperbolic Temporal Graph Attention** We denote hyperbolic TGN in hyperbolic space $\mathbb{L}^{d,K}$ as TGN$N_L$. We build TGN$N_L$ by stacking its sole building block layer, i.e., the hyperbolic temporal graph attention (HypTGA) layer. The HypTGA layer aims to renew node representations at time point $t$, modeling graph dynamics.

As opposed to static graph attention (e.g., GAT) receiving all the neighbors’ features, we conduct aggregation in account of the interaction time between the neighbors. Specifically, for a target node $v_i$ at time $t$, we define its time-aware neighborhood $N_{i,t} = \{v_1, \ldots, v_N\}$ such that the timestamp $t_j$ of the interaction between $v_i$ and $v_j \in N_{i,t}$ is prior to $t$. HypTGA layer takes node representations $h(t)$ and timestamps of node union $\{v_i, \cup N_{i,t}\}$ as the input.

In addition to graph attention, the HypTGA layer further integrates the time encoding $\phi_E(\cdot)$ so that we can distinguish the neighbors in time domain to model graph dynamics. We focus on relative temporal pattern across the neighbors, which remains the same between a shift. Thanks to translation invariance of $\phi_E(\cdot)$, we can encode $t_j = |t - t_j|$ for each neighbor $v_j$ since $|t| - t_j = |t - (t - t_j)|$. Then, we obtain the time-aware representation $\hat{h}_i(t)$ as follows:

$$\hat{h}_i(t) = \phi_L(\hat{t}_j) \otimes^K W \otimes^K h(t),$$

where $\oplus^K$ and $\otimes^K$ are defined before. $\otimes^K$ always has a higher priority than $\oplus^K$, similar to their Euclidean counterparts. As shown in Fig. 1, target node representation $h_i(t)$ is updated by aggregating time-aware representations in $N_{i,t}$.

$$h_i(t) = \text{AGG}^K(\{\alpha_j, \hat{h}_j(t) | j \in \Omega\}), \quad \Omega = i \cup N_{i,t},$$

where we add a self-loop for the target node with $\hat{t}_j = 0$. The attention weight $\alpha_j$ is calculated by the attention function $\text{ATTN}(\cdot, \cdot)$. Naturally, we define $\text{ATTN}(\cdot, \cdot)$ by Lorentzian inner product with a nonlinear activation as follows,

$$\text{ATTN}(\hat{h}_i(t), \hat{h}_j(t)) = h(\gamma(h_i(t), \hat{h}_j(t)) + c),$$

where $\gamma$ and $c$ are weight and bias, respectively. The bias is placed as Lorentzian inner product is restricted in $\mathbb{L}^{d,K}$, i.e., $(x, y) \leq -K$. We define $h(\cdot)$ as $\text{sigmoid}(\cdot)$. Recalling Eq. (15), TGN$N_L$ parameters live in the Euclidean tangent space. Such design will facilitate the model learning.

In TGN$N_L$, for Euclidean input features, we use $\pi_{\mathbb{R}^{d,K}}(\cdot)$ in Eq. (10) to project them onto hyperbolic space $\mathbb{L}^{d,K}$. Meanwhile, we give its Euclidean counterpart, TGN$N_E$. In particular, we utilize Euclidean time encoding $\phi_E(\cdot)$, and replace hyperbolic operators of TGN$N_L$ with Euclidean ones.

**Hyperbolic VGAE**

To model the uncertainty, we introduce a Hyperbolic Variational Graph AutoEncoder (HVGAE) built upon TGN. At the time point $t$, HVGAE infers stochastic representations $z(t)$ of generalized normal distributions with a variational approach in hyperbolic space $\mathbb{L}^{d,K}$. We bridge the gaps of variational approach in hyperbolic space, which are 1) generalizing the (usual) normal distribution, and 2) defining its variational family in hyperbolic space.

**Wrapped Normal Distribution** A canonical approach for generalization is to map a usual normal distribution onto hyperbolic space. Such a probability measure is referred to as wrapped normal distribution (Mathieu et al. 2019). We derive the Probability Density Function (PDF) in $\mathbb{L}^{d,K}$:

$$N^K_{\mathcal{L}}(x | \mu, \text{diag}(\sigma^2)) = F\mathcal{N}(\|P^{\mu\otimes^K}_{\text{diag}(\sigma^2)}(u) - u, \text{diag}(\sigma^2)) \sinh(\frac{\sqrt{K}}{\sqrt{\mathcal{L}}} |u|_{\mathcal{L}})^{1-d},$$

where $F = \left(\frac{1}{\sqrt{K}}\right)^{d-1}$, $u = \log^K(x)$ and $|x|_{\mathcal{L}} = x_{2d+1}$ for $x \in \mathbb{R}^{d+1}$. The wrapped normal distribution owns two

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**Figure 1:** HypTGA Layer. In the time-aware neighborhood, the timestamps $t_1, \ldots, t_4$ are prior to the given time $t$. Einstein midpoint is calculated with the aid of Klein model.
parameters, i.e., a mean $\mu \in \mathbb{L}^{d,K}$ in Lorentz model, and a variance $\sigma \in \mathbb{R}^d$ of a normal distribution $\mathcal{N}(0, \text{diag}(\sigma^2))$ in Euclidean space. The advantage of wrapped normal distribution is that the PDF is differentiable w.r.t. the parameters, so that we can introduce a reparameterisable sampling algorithm, Algorithm 1, to enable the gradient-based learning. Specifically, for a wrapped normal sample, a) we sample a vector from usual normal distribution in Euclidean space (Line 1), b) move the vector to the mean $\mu$ (Line 2 and 3), and c) map it onto hyperbolic space $\mathbb{L}^{d,K}$ (Line 4).

### Hyperbolic Variational Family

In HVGAE, we need to define a prior distribution and the family of corresponding variational posterior in hyperbolic space. In particular, the prior is the standard distribution $\mathcal{N}_L^d(\cdot|0, \mathbf{I})$. The variational family is $\{\mathcal{N}_L^K(\cdot|\mu, \text{diag}(\sigma^2)) | \mu \in \mathbb{L}^{d,K} \}$, where we propose to define the parameters as $\mu = \text{TGNN}_L(G)$ and $\log \sigma = \text{TGNN}_R(G)$. The novelty is two-fold: 1) We define the distribution parameters by the time-aware TGNN, so that the uncertainty is jointly modeled with the dynamics. 2) We introduce a reparameterisable sampling algorithm to enable the gradient-based learning.

### Overall Architecture

Thanks to reparameterisable sampling, HVGNN can be learned in an end-to-end approach with a specific learning task. HVGNN is built with an encoder-decoder framework, illustrated in Fig. 2, and the aforementioned representation learning map $\Phi$ can be defined by the encoder. In particular, we utilize TGNN encoder and a task-oriented decoder. In this paper, we provide the decoder for link prediction and node classification.

#### Encoder

For node $v_i$ at time $t$, we denote the stochastic representation as $z_i(t) \in \mathbb{L}^{d,K}$, summarized in $Z_i$, and denote the class label as $y_i = k \in [1, C]$, summarized in $Y$. With the TGNN encoder, we give the posterior as follows:

$$p(Z_i | G) = \prod_{i=1}^{n} p(z_i(t) | G),$$

where $n$ is the number of nodes in the graph. $q(z_i(t) | G)$ is defined by the hyperbolic variational family above.

#### Decoder

For the task of link prediction, we utilize the Fermi-Dirac decoder. Formally, we have

$$p(G | Z_i) = \prod_{(v_i, v_j) \in E} p((v_i, v_j) \in E | z_i(t), z_j(t)), $$

whose likelihood is defined by the Fermi-Dirac multinomial logistic decoder, formally,

$$p((v_i, v_j) \in E | z_i(t), z_j(t)), $$

where

$$p((v_i, v_j) \in E | z_i(t), z_j(t)),$$

whose likelihood is defined by the Fermi-Dirac multinomial logistic decoder, formally,

$$p((v_i, v_j) \in E | z_i(t), z_j(t)),$$

where

$$p((v_i, v_j) \in E | z_i(t), z_j(t)),$$

whose likelihood is defined by the Fermi-Dirac multinomial logistic decoder, formally,
graphs, i.e., GAT (Veličković et al. 2018) and GraphSAGE (Hamilton, Ying, and Leskovec 2017), and a recent one for dynamic graphs, i.e., TGAT (Xu et al. 2020). Hyperbolic model includes HGCN (Chami et al. 2019), a recent model for static graphs. These methods generate deterministic representations and thereby cannot capture uncertainty.

**Ablation Study** We include the proposed dynamic graph models, i.e., TGN_{NR} and TGN_{NL}, without modeling the uncertainty as baselines. Additionally, we design the Euclidean variant of HVGNN, namely EVGNN, which models dynamic graphs with the uncertainty in Euclidean space. Specifically, we utilize two TGN_{NR} to parameterize usual normal distributions. EVGNN is then optimized with reparameterisable trick of the standard VAE. On the one hand, we can study the importance of modeling uncertainty by comparing HVGNN (EVGNN) against TGN_{NL} (TGN_{NR}). On the other hand, we can study the effect of the representation space by comparing hyperbolic models against their Euclidean counterparts. In the experiment, we stack the corresponding attention layer twice in the models above. Refer Supplementary Material for further experimental details.

**Transductive and Inductive Settings** We evaluate the performances under transductive and inductive settings. Specifically, transductive setting examines output representations of the nodes that have been observed in training. Inductive setting examines output representations of unseen nodes while training. Node representations are initialized as its raw feature. We do chronological train-validation-test split with 80% — 5% — 15% according to the timestamps.

**Link Prediction** The task of link prediction is to predict the probability of two nodes being connected. For hyperbolic models, we utilize the Fermi-Dirac decoder with Lorentz inner product to compute the probability based on the learned representations. For Euclidean models, we replace the Lorentz inner product with normal inner product. The graph models are trained by minimizing the cross-entropy loss using negative sampling. HVGNN owns an additional KL divergence loss to regulate stochastic representations drawn from the wrapped normal distributions. We randomly sample an equal amount of negative node pairs to the positive links, and employ the and classification Accuracy and Average Precision (AP) as evaluation metrics. The performances under transductive and inductive settings are reported in Tables 1 and 2, respectively. The proposed model, HVGNN, consistently outperforms its competitors. For example, on the Wikipedia dataset, HVGNN obtains 3% and 3.64% performance gains against its best competitor in transductive and inductive settings, respectively. The reason is that HVGNN models the inherent characteristics of graphs, i.e., the dynamics and uncertainty, in the promising hyperbolic space. Additionally, we provide further insights though the ablation study: 1) Hyperbolic models (HVGNN and TGN_{NR}) outperform the Euclidean counterparts (EVGNN and TGN_{NL}). This suggests hyperbolic space is a more promising representation space well-suited for modeling real-world graphs. 2) HVGNN and EVGNN achieve better performance than TGN_{NL} and TGN_{NR}, respectively. This shows that the uncertainty cannot be ignored for modeling graphs.
bolic models. We train the comparison models together with the link prediction loss above, encouraging node representations to preserve the graph structure. Owing to the label imbalance on the datasets, we employ the area under the ROC curve (AUC) as the evaluation metric. We summarize the performances under transductive and inductive settings in Table 3. As reported in Table 3, HVGN achieves the best performance consistently. For example, on Wikipedia dataset, HVGN outperforms its best competitor by 2.94% and 3.84% in transductive and inductive settings, respectively. Additionally, the superiority of hyperbolic space and the importance of modeling dynamics and uncertainty are supported in the experimental results.

The Curvature of Hyperbolic Space

In HVGN, we consider the curvature of hyperbolic space, controlled by $K$, as a hyperparameter. In fact, the hyperbolic spaces with different curvatures are essentially the same (Loomis 2013). However, owing to the limited machine precision and normalization, hyperbolic spaces with different curvatures lead to different performances (Chami et al. 2019). For instance, as shown in Figure 3, we obtain performance gain by adjusting the curvature. Motivated by this observation, instead of a fixed curvature, in HVGN, we give the generalized formulation of a trainable curvature to improve its learning capacity.

Table 3: The performance of transductive and inductive node classification in terms of AUC (%).

<table>
<thead>
<tr>
<th>Model</th>
<th>Transductive Setting</th>
<th>Inductive Setting</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Reddit</td>
<td>Wikipedia</td>
</tr>
<tr>
<td>GAT</td>
<td>64.12 ± 0.48</td>
<td>81.54 ± 0.80</td>
</tr>
<tr>
<td>GraphSAGE</td>
<td>60.86 ± 0.59</td>
<td>82.05 ± 0.72</td>
</tr>
<tr>
<td>TGAT</td>
<td>64.88 ± 0.67</td>
<td>83.28 ± 0.56</td>
</tr>
<tr>
<td>HVGN</td>
<td>65.92 ± 0.54</td>
<td>84.55 ± 0.96</td>
</tr>
</tbody>
</table>

Figure 3: The effects of curvature $-1/K$ for inductive learning on Wikipedia dataset.

Conclusion

We have presented a novel HVGN for dynamic graph representation learning in hyperbolic space. HVGN captures graph dynamics and uncertainty in the stochastic representations of wrapped normal distributions in hyperbolic space. HVGN further incorporates a reparameterizable sampling algorithm to enable its gradient-based learning. Experimental results show the superiority of HVGN for link prediction and node classification on several real-world datasets.

Related Work

Graph Representation Learning

Representation learning on graphs is attracting increasing research attentions, and finds itself from network alignment (Sun et al. 2019) to text classification (Peng et al. 2019). Prior works model graphs via random walk (Perozzi, Al-Rfou, and Skiena 2014), or define explicit optimization objectives (Tang et al. 2015; Su et al. 2018). Recent years witness the success of a series of GNNs (Wang, Cui, and Zhu 2016; Ma et al. 2019; Kipf and Welling 2016a). To date, graph modeling is widely studied in static settings while models for dynamic graphs are still scant. Recently, several solutions (Zhou et al. 2018b; Xhonneux, Qu, and Tang 2020) for dynamic graphs are proposed. For example, EvolveGCN (Pareja et al. 2020) models dynamics by formulating a sequence of snapshots. VGRNN (Hajiramezanali et al. 2019) models the uncertainty via an adapted VAE. JODIE (Kumar, Zhang, and Leskovec 2019) models the node trajectories. To our knowledge, all prior models for dynamic graphs consider node representations in Euclidean space, and this is the first model for dynamic graphs in hyperbolic space.

Hyperbolic Representation Learning

Most of representation learning methods assume the representation space to be Euclidean. Actually, hyperbolic space provides an exciting alternative. It is well-suited to model hierarchical or scale-free data (Krioukov et al. 2010; Papadopoulos et al. 2012). An increasing number of studies report hyperbolic model compares favorably to its Euclidean counterpart in a wide spectrum of applications, such as word embedding (Nickel and Kiela 2017; Tifrea, Bećigneul, and Ganea 2019), question answering (Tay, Tuan, and Hui 2018), clustering (Monath et al. 2019), network alignment (Sun et al. 2020) and reasoning in knowledge graph (Balazevic, Allen, and Hospedales 2019). Most of existing methods generate deterministic vectors living hyperbolic space, while some recent works (Mathieu et al. 2019; Nagano et al. 2019) study the generalized normal distributions for stochastic representations. Recently, hyperbolic graph models (Ganea, Bećigneul, and Hofmann 2018; Liu, Nickel, and Kiela 2019) have been proposed where the graph is considered to be static. Distinguishing from these studies, we propose the first hyperbolic model for dynamic graphs.

Figure 3 (a) Link Prediction (b) Node Classification.
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Broad Societal Implications

This paper introduced a novel research problem: dynamic graph representation learning in hyperbolic space. This paper broadens the current graph representation learning research in multiple dimensions, e.g., hyperbolic representation space, dynamic graphs, and stochastic representation learning, to new stages and greatly enriches the current graph neural network studies. This paper possibly motivates further studies on representation learning in the Riemannian manifolds in a more general and elegant way. Furthermore, the model (HVGNN) proposed in this paper has transformative impacts in various real-world applications and a wide spectrum of interdisciplinary studies on graph data, such as online social computing, recommender systems, biomedical studies, and neural science. Both results and source code will be released to the public, and others who otherwise have limited access to the models can use our open-source materials in their researches or applications. We would encourage researchers to explore further applications of our approach, and also welcome the discussion on any theoretical and empirical details, and all kinds of improvements and enhancements from any research field.

References


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