Supplementary material for “Unsupervised Hyperbolic Representation Learning via Message Passing Auto-Encoders”

Jiwoong Park\textsuperscript{1}\textsuperscript{*} Junho Cho\textsuperscript{1} Hyung Jin Chang\textsuperscript{2} Jin Young Choi\textsuperscript{1}
\textsuperscript{1}ASRI, Dept. of ECE, Seoul National University \textsuperscript{2}School of Computer Science, University of Birmingham
\{jtywoong,Junhocho,jychoi\}@snu.ac.kr, h.j.chang@bham.ac.uk

In this supplemental material, we present the reviews of Riemannian geometry and hyperboloid model firstly. Then, we explain the details of the datasets, compared methods, and experimental details. Finally, further experiments on network datasets and further discussions are presented.

1. Riemannian Geometry

1.1. A Review of Riemannian Geometry

A manifold $\mathcal{M}$ of $n$-dimension is a topological space that each point $x \in \mathcal{M}$ has a neighborhood that is homeomorphic to $n$-dimensional Euclidean space $\mathbb{R}^n$. For each point $x \in \mathcal{M}$, a real vector space $T_x \mathcal{M}$ whose dimensionality is the same as $\mathcal{M}$ exists and is called a tangent space. The tangent space $T_x \mathcal{M}$ is the set of all the possible directions and speeds of the curves on $\mathcal{M}$ across $x \in \mathcal{M}$. A Riemannian manifold is a tuple $(\mathcal{M}, g)$ that is possessing Riemannian metric $g_x : T_x \mathcal{M} \times T_x \mathcal{M} \rightarrow \mathbb{R}$ on the tangent space $T_x \mathcal{M}$ at each point $x \in \mathcal{M}$ such that $\langle y, z \rangle_x = g_x(y, z) = y^T G(x) z$, where $G(x)$ is a matrix representation of Riemannian metric $[27]$. The metric tensor provides geometric notions such as the length of curve, angle and volume. The length of curve $\gamma : t \mapsto \gamma(t) \in \mathcal{M}$ is $L(\gamma) = \int_0^1 \| \gamma'(t) \|_{\gamma(t)} dt$. The geodesic, the generalization of straight line on Euclidean space, is the constant speed curves giving the shortest path between the pair of points $x, y \in \mathcal{M}$: $\gamma^* = \arg \min_{\gamma} L(\gamma)$ where $\gamma(0) = x$, $\gamma(1) = y$ and $\| \gamma'(t) \|_{\gamma(t)} = 1$. The global distance between two points $x, y \in \mathcal{M}$ is defined as $d_\mathcal{M}(x, y) = \inf_{\gamma} L(\gamma)$.

1.2. Hyperboloid Model

The hyperbolic space is a Riemannian manifold with constant negative sectional curvature equipped with hyperbolic geometry, and the hyperboloid model is one of the multiple equivalent hyperbolic models. For $x, y \in \mathbb{R}^{n+1}$, the Lorentz inner product $\langle x, y \rangle_{\mathbb{L}}$ is defined as $\langle x, y \rangle_{\mathbb{L}} = -x_0 y_0 + \sum_{i=1}^{n} x_i y_i$. The $n$-dimensional hyperboloid with constant negative curvature $K(K < 0)$ is defined as $(\mathbb{H}_K^n, g_K^n)$:

$$\mathbb{H}_K^n = \{ x \in \mathbb{R}^{n+1} : \langle x, x \rangle_{\mathbb{L}} = 1/K, x_0 > 0 \}. \quad (1)$$

The metric tensor is $g_{\mathbb{H}_K^n} = \text{diag}(\{−1, 1, \ldots, 1\})$, and the origin of the hyperboloid model is $o = (1/\sqrt{|K|}, 0, \ldots, 0) \in \mathbb{R}^{n+1}$. The distance between two points $x, y \in \mathbb{H}_K^n$ is defined as

$$d_{\mathbb{H}_K^n}(x, y) = \frac{1}{\sqrt{-K}} \arccosh(\langle x, y \rangle_{\mathbb{L}}). \quad (2)$$

For points $x \in \mathbb{H}_K^n$, tangent vector $v \in T_x \mathbb{H}_K^n$, and $y \neq 0$, $\exp_x : T_x \mathbb{H}_K^n \rightarrow \mathbb{H}_K^n$ and $\log_x : \mathbb{H}_K^n \rightarrow T_x \mathbb{H}_K^n$ are defined as

$$\exp_K^x(v) = \cosh(s)x + \sinh(s)\frac{v}{s}, \quad (3)$$

$$\log_K^x(y) = \frac{\arccosh(\langle K(x, y) \rangle_{\mathbb{L}})}{\sqrt{K^2 \langle x, y \rangle_{\mathbb{L}}^2 - 1}} (y - K \langle x, y \rangle_{\mathbb{L}} x), \quad (4)$$

where $s = \sqrt{-K\|v\|_{\mathbb{L}}^2}$ and $\|x\|_{\mathbb{L}} = \sqrt{\langle x, x \rangle_{\mathbb{L}}}$.

2. Datasets

2.1. Network Datasets

Phylogenetic tree [14, 32] models the generic heritage. CS PhDs [10] represents the relationship between Ph.D. candidates and their advisors in computer science fields. Diseases [12, 30] is a biological network expressing the relationship between diseases. Cora [33], Citeseer [33], Pubmed [33], and Wiki [41] are citation networks whose nodes are scientific papers or web pages and edges represent citation relationships between any two papers or links.

\textsuperscript{*}equally contributed.

\textsuperscript{1}http://hyperbolicedeeplearning.com/simple-geometry-initiation/
between any two web pages. BlogCatalog [35] models a social network among bloggers in the online community. Attribute and label of a node represent the description of each blog and the interest of a blogger, respectively. Amazon Photo [23] is a part of Amazon co-purchase networks whose nodes are goods and edges represent purchase correlations between any two goods. A node attribute indicates the bag-of-words for goods’ reviews and its label denotes a product category.

2.2. Image Datasets

ImageNet-10 [7] and ImageNet-Dogs [7] are subsets of the ImageNet dataset [19]. ImageNet-10 consists of 13,000 images from 10 randomly selected subjects. ImageNet-Dogs are 19,500 images from 15 randomly selected dog breeds. The class hierarchy of ImageNet-Dogs is illustrated in Fig. 1. We have constructed a new dataset, ImageNet-BNCR, via randomly choosing 3 leaf classes per root. We chose three roots, Artifacts, Natural objects, and Animal. Thus, there exist 9 leaf classes, and each leaf class contains 1,300 images in ImageNet-BNCR dataset. For every dataset used for the image clustering task, we used only the training set without the validation set, and images were resized to 96 × 96 × 3.

3. Compared Methods

3.1. Node Clustering and Link Prediction

We compared HGCAE with seven state-of-the-art unsupervised message passing models which mainly conduct in Euclidean space.

- GAE [18], VGAE [18], ARGA [25], and ARVGA [25] are graph auto-encoders that reconstruct only the affinity matrix using a non-parametric decoder which is not learnable.

- MGAE [38] is a stacked one-layer graph auto-encoder that reconstructs only the node attributes via a linear activation function.

- GALA [26] is a graph auto-encoder that reconstructs only the node attributes through learnable parametric encoder and decoder.

- DBGAN [47] is a distribution-induced bidirectional generative adversarial network that estimates the structure-aware prior distribution of the representations.

GAE [18], VGAE [18], ARGA [25], ARVGA [25], and GALA [26] are constrained to have two-layer auto-encoder models, since they report that two-layer structures show the best performances. In the case of MGAE [38] which is a stacked one-layer auto-encoder model, we have stacked the layer up to three and reported the best performances. For
model convergence. During training for the link prediction task, we only reconstructed training edges in $L_{REC-A} = \mathbb{E}_{q(H|X,A)}[\log p(A|H)]$. For the node clustering task, every edge is reconstructed by the output of the encoder during training. The performance of node clustering was obtained by running k-means clustering [21] on the latent representations (output of the encoder) in the tangent space of the last layer of the encoder.

4.2. Details of Image Clustering

The performance of HGCAE on the image clustering task was obtained by running k-means clustering [21] on the latent representations (output of the encoder) in the tangent space of the last layer of the encoder.

4.3. Details of Convolutional Auto-Encoder

We extracted 1000-dimensional features by training a convolutional auto-encoder (CAE) [22] on the ImageNet-10 [7] and ImageNet-BNCR datasets on the experiment of Section 5.3 in the manuscript. We used the encoder part and decoder part as VGG-16 network [34] and five deconvolution layers [44] respectively. We optimized CAE using Adam [16] with learning rate 0.0001 and obtained the feature after 100 epochs.

4.4. Details of Image Classification

We obtained the latent representation of ImageNet-10 [7] and ImageNet-BNCR by training CAE on the experiments of Section 5.4 in the manuscript. For the image classification task, we trained the VGG-11 [34] classifier. We trained the classifier using stochastic gradient descent [3] and used the learning rate scheduler as in [43]. When adding further samples in every training epoch, high, middle, and low HDO samples were chosen by $n\%$ of the original data closest to the boundary, $n\%$ of the original data closest to the median of distance histogram, and $n\%$ of the original data closest to the origin, respectively. We set $n$ for ImageNet-10 and ImageNet-BNCR to 30 and 50 respectively. The learning rates of ImageNet-10 and ImageNet-BCNR were set to 0.01 and 0.0005 respectively. When training BaselineFL, we tried $\{0.5, 1.0, 2.0\}$ for $\gamma$ in focal loss [20] and reported the best performances. There has been recent research on manipulating the gradient updates based on the prediction difficulty, anchor loss (AL) [31], and we have tried to report the classification performance of AL as well as FL. However, due to the several NaN issues of official AL implementation\(^3\), we could not report the performance of AL.

5. Further Experiments

5.1. Effectiveness of The Proposed Components

Through link prediction experiments, we validated the effectiveness of two components: learning in the hyperbolic

\(^3\)https://github.com/alr-you41/AnchorLoss
Table 1: Ablation studies on link prediction task: The baseline model is GAE which conducts graph convolution in Euclidean space, does not use an attention mechanism and reconstructs only the graph structure $A$.

|                  | Reconstruct both $A$ and $X$ | Geometry aware attention | in hyperbolic space fixing $K$ | in hyperbolic spaces learning $K$ | Cora AUC | Cora AP | Citeseer AUC | Citeseer AP |
|------------------|------------------------------|--------------------------|--------------------------------|----------------------------------|--------|--------|-------------|-------------|
| Baseline: GAE [18] | ×                            | ×                        | ×                              | ×                                | 91.0   | 92.0   | 89.5        | 89.9        |
| Ablation I       | ✓                            | ×                        | ✓                              | ×                                | 92.7   | 92.1   | 94.0        | 94.8        |
| Ablation II      | ✓                            | ✓                        | ✓                              | ✓                                | 94.6   | 94.4   | 95.9        | 96.3        |
| Ablation III     | ×                            | ✓                        | ✓                              | ✓                                | 94.5   | 94.8   | 96.1        | 96.4        |
| Proposed I: HGCAE| ✓                            | ✓                        | ✓                              | ×                                | 95.4   | 95.5   | 96.7        | 97.0        |
| Proposed II: HGCAE| ✓                            | ✓                        | ×                              | ✓                                | 95.6   | 95.5   | 96.5        | 96.8        |

Table 2: Clustering performances in low-dimensional space.

|          | Pubmed | BlogCatalog | Amazon Photo |
|----------|--------|-------------|--------------|
| GAE [18] | 51.3   | 7.7         | 27.6         |
| VGAE [18]| 40.6   | 0.1         | 23.3         |
| ARG [25] | 40.0   | 0.5         | 29.8         |
| ARG [25] | 38.5   | 0.1         | 27.2         |
| GALA [26]| 36.1   | 0.4         | 25.2         |
| HGCAE    | 68.1   | 28.2        | 74.1         |

5.2. Learning in Low-Dimensional Space

One of the strengths of hyperbolic space compared to Euclidean space is that hyperbolic model can learn latent representation of data whose structure is hierarchical without the need for infeasible high-dimensional space [11]. To show this point, we obtained the latent representations of network datasets in the very low-dimensional latent space for node clustering task. Every compared graph autoencoder and HGCAE were constrained to have two layers whose each dimension was 4 and 2 respectively. Note that the performance of MGAE [38] cannot be reported since MGAE cannot manipulate the latent dimension. The experiments were conducted on Pubmed [33], BlogCatalog [35], and Amazon Photo [23] datasets. The results are presented in Table 2. Although the dimension of latent space is extremely low, HGCAE still significantly outperforms the

Figure 2: 2-dimensional embeddings in Euclidean, Poincaré ball, and hyperboloid latent spaces on Pubmed, BlogCatalog, Citeseer, and Amazon Photo datasets.
state-of-the-art unsupervised message passing methods operating in Euclidean space. Notably, on BlogCatalog and Amazon Photo datasets, HGCAE achieves more than 30% higher performances compared to Euclidean counterparts. These results support that hyperbolic space is effective than Euclidean space even in the very low-dimensional latent space.

5.3. Visualization of The Network Datasets

We explored the latent representations of GAE [18] and our models on Pubmed [35], BlogCatalog [35], Citeseer [33], and Amazon Photo [23] datasets by constraining the latent space as a 2-dimensional hyperbolic or Euclidean space. The result is given in Fig. 2. On the results of HGCAE, most of the nodes are located on the boundary of hyperbolic space and well-clustered with the nodes in the same class.

5.4. Sensitivity of Hyperparameter Setting

One of the important hyperparameters of HGCAE is $\lambda$ in Eq. (12) in the manuscript. If $\lambda$ is required large (small) value, this means that the node attributes (subgraph structures) are the more important factor of latent representation. Since node attributes and the graph structure are different for each dataset, the optimal $\lambda$ has different values for each dataset. In cases of BlogCatalog and Citeseer (Cora), we empirically found that small (large) $\lambda$ value is optimal for both link prediction and node clustering tasks.

6. Further Discussions

6.1. Connection to Contrastive Learning

The hyperbolic geometry can be extended to contrastive learning [8]. A recent study [36] has uncovered the link between contrastive learning and deep metric learning. In this respect, it is becoming more significant to find the informative (hard) negative samples, embeddings that are difficult to distinguish from anchors, beyond uniform sampling [29]. Our work empirically showed that Hyperbolic Distance from the Origin (HDO) is an effective criterion for selecting samples without supervision for better generalization. The concept of HDO could be extended to informative negative sampling. Since the embeddings hard to discriminate is equal to those that are hard to classify by the model, the samples near the origin of hyperbolic space can be the impactful negative samples to increase the ability of the un-supervised contrastive learning.

6.2. Failure Cases of Hyperbolic Embedding Spaces

The inductive bias of hyperbolic representation learning is assuming that there exist hierarchical relationships in the dataset. Thus if the structure of the graph modeling the relation between data points is close to a tree, the hyperbolic space, a continuous version of a tree, is a suitable latent space. However, not all datasets’ latent structures have the topological properties of the tree. For instance, datasets obtained from omnidirectional sensors of drones and autonomous cars are indeed more suitable to latent hyperspherical manifold rather than the hyperbolic manifold [9].

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