Representation Learning with Weighted Inner Product for Universal Approximation of General Similarities

Geewook Kim 1,2, Akifumi Okuno 1,2, Kazuki Fukui 1,2, and Hidetoshi Shimodaira 1,2

1Graduate School of Informatics, Kyoto University, 36-1 Yoshida Honmachi, Sakyo-ku, Kyoto, Japan
2RIKEN Center for Advanced Intelligence Project (AIP), 1-4-1 Nihonbashi, Chuo-ku, Tokyo, Japan

Abstract

We propose weighted inner product similarity (WIPS) for neural-network based graph embedding, where we optimize the weights of the inner product in addition to the parameters of neural networks. Despite its simplicity, WIPS can approximate arbitrary general similarities including positive definite, conditionally positive definite, and indefinite kernels. WIPS is free from similarity model selection, yet it can learn any similarity models such as cosine similarity, negative Poincaré distance and negative Wasserstein distance. Our extensive experiments show that the proposed method can learn high-quality distributed representations of nodes from real datasets, leading to an accurate approximation of similarities as well as high performance in inductive tasks.

1. Introduction

Representation learning of graphs, also known as graph embedding, computes vector representations of nodes from graph structured data. The learned representations called feature vectors are widely-used in a range of applications, e.g., community detection and link prediction in social networks (Tang et al., 2015; Hamilton et al., 2017). Words in a text corpus also constitute a co-occurrence graph, and the learned feature vectors of words are successfully applied in many natural language processing tasks (Mikolov et al., 2013).

The feature vector is a model parameter or computed from node’s attributes called data vector. Many of state-of-the-art graph embedding methods train feature vectors in low dimensional Euclidean space so that their inner product expresses the similarity representing the strength of association between nodes. This common framework is referred to as inner product similarity (IPS) in this paper. IPS equipped with a sufficiently large neural network is highly expressive and it has been proved to approximate arbitrary Positive Definite (PD) similarities (Okuno et al., 2018a), e.g., cosine similarity. However, IPS cannot express non-PD similarities.

Naturally, similarity functions based on specific kernels other than inner product have been considered. For instance, hierarchical structure of words is well represented in hyperbolic space with Poincaré distance (Nickel and Kiela, 2017). Whereas practitioners are required to specify a latent similarity model for representation learning on a given data, finding the
best model is not a simple problem, leading to a tedious trial and error process. To address this issue, we need a highly expressive similarity model.

Recently, a simple similarity model named \textit{shifted inner product similarity (SIPS)} has been proposed by introducing bias terms in IPS model (Okuno et al., 2018b). SIPS can approximate arbitrary conditionally PD (CPD) similarities, which includes any PD similarities and many other widely-used similarities, e.g., negative Poincaré distance and negative Wasserstein distance. However, the approximation capability of SIPS is still limited to CPD similarities.

To further enhance the approximation capability of IPS model, \textit{inner product difference similarity (IPDS)} has been proposed by taking the difference between two IPS models (Okuno et al., 2018b, See Supplement E). Any general similarities including indefinite kernels can be expressed as the difference between two PD similarities (Ong et al., 2004), thus they can be approximated by IPDS arbitrarily well. However, only the concept of IPDS has been shown without conducting any experiments there.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Proposed WIPS is capable of approximating any general similarities, including PD, CPD and a variety of other similarities.}
\end{figure}

In this paper, we examine IPDS on a range of applications to investigate its effectiveness and weakness. There are practical concerns such as specification of dimensionalities of the two IPS models. In order to remedy the weakness of IPDS, we propose a new model named \textit{weighted inner product similarity (WIPS)}. The core idea of WIPS is to incorporate element-wise weights to IPS so that it generalizes all the above-explained similarity models. WIPS reduces to IPS when all the weights are +1, and it also reduces to IPDS when they are +1 or −1. The weight values are optimized continuously by allowing positive and negative values, and thus WIPS is free from model selection, except for the choice of dimensionality. Through our extensive experiments, we verify the efficacy of WIPS in real-world applications.

Our contributions for representation learning are: (i) A new model WIPS is proposed for universal approximation of general similarities without model selection. (ii) Experiments of WIPS as well as IPDS are conducted for showing their high approximation capabilities. (iii) All of our implementations with experimental code will be publicly available.

2. Related Works

In this section, we overview some existing methods concerned with similarity learning.

\textbf{Metric learning} is a kind of similarity learning where similarity between two data vectors $x_i, x_j$ is captured by some metric function $d(x_i, x_j)$ (Bellet et al., 2013; Kulis et al., 2013). A vast amount of previous works focused on linear metric learning, where
Mahalanobis distance $d_M(x_i, x_j) = \sqrt{(x_i - x_j)^\top M (x_i - x_j)}$ is trained with respect to positive-semidefinite (PSD) matrix $M$. Finding such a PSD matrix $M$ in this context is interpreted as finding a linear projection $L$ that transforms each data vector by $L^\top x$ (Goldberger et al., 2005), since the PSD matrix $M$ can be decomposed as $M = LL^\top$. Therefore, it can also be seen as learning linear embedding so that similar feature vectors get closer. It is extended to learning non-linear transformation by replacing $L$ with neural networks, which has been known as Siamese architecture (Bromley et al., 1994). When it comes to just capturing the similarities, especially with bilinear form of $x_i^\top M x_j$, $M$ no longer needs to be PSD (Chechik et al., 2009); these non-metric learning methods are closely related to our non-PD similarities, but they do not learn embedding representations of data vectors.

Kernel methods represent similarity between two data vectors by a positive-definite (PD) kernel. Although the similarity can be shown as the inner product associated with Reproducing Kernel Hilbert Space (RKHS), explicit embedding representations of data vectors are avoided via the kernel trick. Kernel methods have been extended to conditionally PD (CPD) kernels (Schölkopf, 2001) for representing negative distances, and also to general kernels including indefinite kernels (Ong et al., 2004; Oglic and Gaertner, 2018) for representing a variety of non-PD kernels in real-world situations (Schleif and Tino, 2015). The general kernels are theoretically expressed as inner products associated with Reproducing Kernel Krĕın Space (RKKS), but such representations in infinite dimensions are avoided in practice.

Graph embedding can be interpreted as learning representations of nodes that preserve similarities between nodes defined from their links or neighbourhood structure. The feature vector of a node is computed from its data vector using linear transformation (Yan et al., 2007) or non-linear transformation (Wang et al., 2016), whereas feature vectors are treated as model parameters when data vectors are not observed (Tang et al., 2015). Word embedding with skipgram model (Mikolov et al., 2013) in natural language processing can also be interpreted as graph embedding without data vectors. They are often 2-view graphs, where vector representations of words and those of contexts are parameterized separately. Some graph embedding methods implement such 2-view settings (Tang et al., 2015), and its generalization to a multi-view setting is straightforward (Okuno et al., 2018a). Interestingly, most of these graph embedding models implement the inner product for computing similarity, thus they can be covered by our argument, although we work only on a 1-view case just for simplicity of notation. Note that graph convolution networks (Hamilton et al., 2017) compute the feature vector of a node from the data vectors of its neighbour nodes, so they cannot be covered by our simple setting. However, these methods also use inner product, thus they may be improved by using our similarity models.

3. Representation Learning for Graph Embedding

Let us consider an undirected graph consisting of $n(\in \mathbb{N})$ nodes $\{v_i\}_{i=1}^n$ with weighted adjacency matrix $(w_{ij})_{i,j=1}^n \in \mathbb{R}_{\geq 0}^{n \times n}$. The symmetric weight $w_{ij} = w_{ji} \geq 0$ is called link weight, that represents the observed strength of association between node pair $(v_i, v_j)$ for all $1 \leq i < j \leq n$. We may also consider a data vector $x_i \in \mathcal{X}$ at $v_i$, that takes value in a set $\mathcal{X} \subset \mathbb{R}^p (p \in \mathbb{N})$. The data vector represents attributes or side-information at the node. If we do not have any such attributes, we use 1-hot vector instead, i.e., $x_i$ is $n$-dimensional
vector whose \(i\)-th entry is 1 and 0 otherwise, for \(i = 1, \ldots, n\). Our data consists of \(\{w_{ij}\}_{i,j=1}^n\) and \(\{x_i\}_{i=1}^n\).

Following the setting of graph embedding described in Okuno et al. (2018a,b), we consider a feature vector \(y_i \in Y\) at \(v_i\), that takes value in a set \(Y \subset \mathbb{R}^K\) for some dimensionality \(K \in \mathbb{N}\). Feature vectors are computed by a continuous transformation \(f : \mathcal{X} \to \mathcal{Y}\) as

\[
y_i := f(x_i) \quad (i = 1, 2, \ldots, n).
\]

For two data vectors \(x, x' \in \mathcal{X}\), the strength of association between \(x\) and \(x'\) is modeled by a similarity function

\[
h(x, x') := g(f(x), f(x')),
\]

where \(g : Y^2 \to \mathbb{R}\) is a symmetric continuous function, e.g., the inner product \(g(y, y') = \langle y, y' \rangle = \sum_{k=1}^{K} y_k y'_k\). We employ a simple random graph model by specifying the conditional expectation of \(w_{ij}\) given \(x_i\) and \(x_j\) as

\[
E(w_{ij}|x_i, x_j) = \nu(h(x_i, x_j; \theta, \lambda)),
\]

where \(\nu : \mathbb{R} \to \mathbb{R}\) is a non-linear function; e.g., \(\nu(x) = \sigma(x) := (1 + \exp(-x))^{-1}\) is sigmoid function when \(w_{ij} \in \{0, 1\}\) follows Bernoulli distribution, or \(\nu(x) = \exp(x)\) when \(w_{ij} \in \{0, 1, \ldots\}\) follows Poisson distribution.

For learning distributed representations of nodes from the observed data, we consider a parametric model \(f_\theta : \mathcal{X} \to \mathcal{Y}\) with unknown parameter vector \(\theta \in \Theta\). Typically, \(f_\theta\) is a non-linear transformation implemented as a vector valued neural network (NN), or a linear transformation. The similarity function \(h\) is now modelled as

\[
h(x, x'; \theta, \lambda) := g_\lambda(f_\theta(x), f_\theta(x')),
\]

where \(g_\lambda(y, y')\) has also a parameter vector \(\lambda\) in general. This architecture for similarity learning is called Siamese network (Bromley et al., 1994). The parameter \(\theta \in \Theta\) as well as \(\lambda\) may be estimated by maximizing the log-likelihood function. For the case of Bernoulli distribution (i.e., the binary \(w_{ij}\)), the objective function is

\[
\sum_{1 \leq i < j \leq n} w_{ij} \log \nu(h(x_i, x_j; \theta, \lambda))
+ \sum_{1 \leq i < j \leq n} (1 - w_{ij}) \log(1 - \nu(h(x_i, x_j; \theta, \lambda)))
\]

which is optimized efficiently by mini-batch SGD with negative sampling (Okuno et al., 2018a). Once the optimal parameters \(\theta\) and \(\lambda\) are obtained, we compute feature vectors as \(y_i = f_\theta(x_i), i = 1, \ldots, n\). For inductive tasks with newly observed data vectors \(x_i\) \((i = n + 1, n + 2, \ldots)\), we also compute feature vectors by \(y_i = f_\theta(x_i)\) unless \(x_i\) are 1-hot vectors, and then we can compute similarity function \(g_\lambda(y_i, y_j)\) for any pair of feature vectors.
4. Existing Similarity Models and Their Approximation Capabilities

The quality of representation learning relies on the model (1) of similarity function. Although arbitrary similarity functions can be expressed if $g_\lambda$ is a large neural network with many units, our $g_\lambda$ are confined to simple extensions of inner product in this paper. All the models reviewed in this section are very simple and they do not have the parameter $\lambda$. You will see very subtle extensions to the ordinary inner product greatly enhance the approximation capability.

4.1 Inner Product Similarity (IPS)

Many of conventional representation learning methods use IPS as its similarity model. IPS is defined by

$$h_{\text{IPS}}(x, x'; \theta) = \langle f_\theta(x), f_\theta(x') \rangle,$$

where $\langle y, y' \rangle = \sum_{k=1}^K y_k y_k'$ represents the inner product in Euclidean space $\mathbb{R}^K$. Note that, $h_{\text{IPS}}(x, x'; \theta)$ reduces to Mahalanobis inner product $x^\top L_\theta L_\theta^\top x'$ (Kung, 2014), by specifying $f_\theta(x)$ as a linear-transformation $L_\theta x$ with a matrix $L_\theta \in \mathbb{R}^{p \times K}$ parameterized by $\theta \in \Theta$. For describing the approximation capability of IPS, we need the following definition.

**Definition 4.1 (Positive definite kernel)** A symmetric function $h : \mathcal{X}^2 \to \mathbb{R}$ is said to be positive-definite (PD) if $\sum_{i=1}^n \sum_{j=1}^n c_i c_j h(x_i, x_j) \geq 0$ for any $\{x_i\}_{i=1}^n \subset \mathcal{X}$ and $\{c_i\}_{i=1}^n \subset \mathbb{R}$. This definition of PD includes positive semi-definite. Note that $h$ is called negative definite when $-h$ is positive definite.

For instance, $h(x, x') = g(f(x), f(x'))$ is PD when $g(y, y') = \langle y, y' \rangle$ (IPS), and $g(y, y') = \langle y, y' \rangle/\|y\|_2\|y'\|_2$ (cosine similarity).

IPS using a sufficiently large NN has been proved to approximate arbitrary PD similarities (Okuno et al., 2018a, Theorem 3.2), in the sense that, for any PD-similarity $h_*$, $h_{\text{IPS}}(x, x'; \theta)$ equipped with a NN converges to $h_*(x, x')$ as the number of units in the NN and the dimension $K$ increase. The theorem is proved by combining the universal approximation theorem of NN (Funahashi, 1989; Cybenko, 1989; Yarotsky, 2017; Telgarsky, 2017), and the Mercer’s theorem (Minh et al., 2006). Therefore, IPS, despite its simplicity, covers a very large class of similarities. However, IPS cannot approximate non-PD similarities (Okuno et al., 2018b), such as the negative-squared distance $h(x, x') = -\|f(x) - f(x')\|_2^2$.

4.2 Shifted Inner Product Similarity (SIPS)

For enhancing the IPS’s approximation capability, Okuno et al. (2018b) has proposed shifted inner product similarity (SIPS) defined by

$$h_{\text{SIPS}}(x, x'; \theta) = \langle \tilde{f}_\theta(x), \tilde{f}_\theta(x') \rangle + u_\theta(x) + u_\theta(x'),$$

where $\tilde{f}_\theta : \mathcal{X} \to \mathbb{R}^{K-1}$ and $u_\theta : \mathcal{X} \to \mathbb{R}$ are continuous functions parameterized by $\theta$. Thus $f_\theta(x) = (\tilde{y}, z) := (\tilde{f}_\theta(x), u_\theta(x)) \in \mathbb{R}^K$ represents the feature vector for $x$. By introducing the bias terms $u_\theta(x) + u_\theta(x')$, SIPS extends the approximation capability of IPS.

For describing the approximation capability of SIPS, we need the following definition.
Definition 4.2 (Conditionally positive definite kernel) A symmetric function \( h : \mathcal{X}^2 \to \mathcal{R} \) is said to be conditionally \( PD \) (CPD) if \( \sum_{i=1}^{n} \sum_{j=1}^{n} c_{ij} h(x_i, x_j) \geq 0 \) for any \( \{x_i\}_{i=1}^{n} \subset \mathcal{X} \) and \( \{c_i\}_{i=1}^{n} \subset \mathcal{R} \) satisfying \( \sum_{i=1}^{n} c_{i} = 0 \).

CPD includes many examples, such as any of PD similarities, negative squared distance, negative Poincaré distance used in Poincaré embedding (Nickel and Kiela, 2017) and some cases of negative Wasserstein distance (Xu et al., 2018).

SIPS using a sufficiently large NN has been proved to approximate arbitrary CPD similarities (Okuno et al., 2018a, Theorem 4.1). Therefore, SIPS covers even larger class of similarities than IPS does. However, there still remain non-CPD similarities (Okuno et al., 2018a, Supplement E.3) such as negative Jeffrey’s divergence and Epanechnikov kernel.

4.3 Inner Product Difference Similarity (IPDS)

For further enhancing the SIPS’s approximation capability, Okuno et al. (2018b) has also proposed inner-product difference similarity (IPDS). By taking the difference between two IPSs, we define IPDS by

\[ h_{IPDS}(x, x'; \theta) = \langle f_{\theta}^+(x), f_{\theta}^+(x') \rangle - \langle f_{\theta}^-(x), f_{\theta}^-(x') \rangle, \]

where \( f_{\theta}^+: \mathcal{X} \to \mathcal{R}^{K-q} \) and \( f_{\theta}^-: \mathcal{X} \to \mathcal{R}^{q} \) \((0 \leq q \leq K)\) are continuous functions parameterized by \( \theta \in \Theta \). Thus \( f_{\theta}(x) = (y^+, y^-) := (f_{\theta}^+(x), f_{\theta}^-(x)) \in \mathcal{R}^K \) represents the feature vector for \( x \). SIPS with \( K \) dimensions is expressed as IPDS with \( K + 2 \) dimensions by specifying \( f^+(x) = (\tilde{f}_\theta(x), u_\theta(x), 1) \in \mathcal{R}^{K+1} \) and \( f^-(x) = u_\theta(x) - 1 \in \mathcal{R} \). Therefore, the class of similarity functions of IPDS includes that of SIPS. Also note that IPDS with \( q = 1 \) and constraint \( h_{IPDS}(x, x; \theta) = -1 \) gives the bilinear form in the hyperbolic space, which is used as another representation for Poincaré embedding (Nickel and Kiela, 2018; Leimeister and Wilson, 2018). For vectors \( y_i = (y_i^+, y_i^-) \), the bilinear-form \( \langle y_i^+, y_j^+ \rangle - \langle y_i^-, y_j^- \rangle \) is known as an inner product associated with pseudo-Euclidean space (Greub, 1975), which is also said indefinite inner product space, and such inner products have been used in applications such as pattern recognition (Goldfarb, 1984).

For describing the approximation capability of IPDS, we need the following definition.

Definition 4.3 (Indefinite kernel) A symmetric function \( h : \mathcal{X}^2 \to \mathcal{R} \) is said to be indefinite if neither of \( h \) nor \(-h\) is positive definite. We only consider \( h \) which satisfies the condition

\[ h' - h \text{ is PD for some PD kernel } h', \]

so that \( h \) can be decomposed as \( h = h_1 - h_2 \) with two PD kernels \( h_1 \) and \( h_2 \) (Ong et al., 2004, Proposition 7).

We call \( h \) general similarity function when \( h \) is positive definite, negative definite, or indefinite.

IPDS using a sufficiently large NN (with many units, large \( K - q \) and \( q \)) has been proved to approximate arbitrary general similarities (Okuno et al., 2018a, Theorem E.1), thus IPDS should cover an ultimately large class of similarities.
4.4 Practical Issues of IPDS

Although IPDS can universally approximate any general similarities with its high approximation capability, only the theory of IPDS without any experiments nor applications has been presented in previous research (Okuno et al., 2018b). There are several practical concerns when IPDS is implemented. The optimization of $f_\theta$ for IPDS can be harder than IPS and SIPS without proper regularization, because the expression of IPDS is redundant; for arbitrary $f_\theta^0$, replacing $f_\theta^0(x)$ with $(f_\theta^0(x), f_\theta^0(x))$, respectively, results in exactly the same similarity model but with redundant dimensions. Choice of the two dimensionalities, i.e., $K - q$ and $q$, should be important. This leads to our development of new similarity model presented in the next section.

5. Proposed Similarity Model

We have seen several similarity models which can be used as a model of (1) for representation learning in graph embedding. In particular, IPDS has been mathematically proved to approximate any general similarities, but choice of the two dimensionalities can be a practical difficulty. In order to improve the optimization of IPDS, we propose a new similarity model by modifying IPDS slightly. Everything is simple and looks trivial, yet it works very well in practice.

5.1 Weighted Inner Product Similarity (WIPS)

We first introduce the inner product with weights.

**Definition 5.1 (Weighted inner product)** For two vectors $y = (y_1, y_2, \ldots, y_K), y' = (y'_1, y'_2, \ldots, y'_K) \in \mathbb{R}^K$, weighted inner product (WIP) equipped with the weight vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_K) \in \mathbb{R}^K$ is defined as

$$\langle y, y' \rangle_\lambda := \sum_{k=1}^{K} \lambda_k y_k y'_k.$$ 

The weights $\{\lambda_k\}_{k=1}^K$ may take both positive and negative values in our setting; thus, WIP is an indefinite inner product (Böttcher and Lancaster, 1996).

WIP reduces to the ordinary inner product $\langle y, y' \rangle$ when $\lambda = 1_K := (1, 1, \ldots, 1) \in \mathbb{R}^K$. WIP also reduces to the indefinite inner product $\langle y_i^+, y_j^+ \rangle - \langle y_i^-, y_j^- \rangle$ when $\lambda = (1, \ldots, 1, -1, \ldots, -1) = (1_K - q, -1_q) \in \mathbb{R}^K$.

For alleviating the problem to choose appropriate value of $q$ in IPDS, we propose weighted inner product similarity (WIPS) defined by

$$h_{\text{WIPS}}(x, x'; \theta, \lambda) = \langle f_\theta(x), f_\theta(x') \rangle_\lambda,$$

where $f_\theta : \mathbb{R}^p \rightarrow \mathbb{R}^K$ is a non-linear transformation parameterized by $\theta \in \Theta$, and $\lambda \in \mathbb{R}^K$ is also a parameter vector to be estimated. The parameter vectors $\theta$ and $\lambda$ are jointly optimized in the objective function (2). WIPS obviously includes IPS, SIPS, and IPDS as special cases by specifying $\lambda$ and $f_\theta$ (Table 1). WIPS inherits the universal approximation.
capability of general similarities from IPDS, but WIPS does not extend IPDS for a larger class of similarity functions; WIPS is expressed as IPDS by redefining $f_{\theta}$ so that $k$-th element is rescaled by $\sqrt{\lambda_k}$ for $\lambda_k > 0$ and $\sqrt{-\lambda_k}$ for $\lambda_k < 0$. However, the discrete optimization of $0 \leq q \leq K$ in IPDS is mitigated by the continuous optimization of $\lambda \in \mathbb{R}^K$ in WIPS.

| WIPS      | $\lambda$     | $f_{\theta}$                          |
|-----------|---------------|----------------------------------------|
| IPS       | $1_K$         | $f_{\theta}$                           |
| SIPS      | $(1_{K+1}, -1)$| $(\tilde{f}_{\theta}(x), u_{\theta}(x), 1, u_{\theta}(x) - 1)$ |
| IPDS      | $(1_{K-q}, -1_q)$| $(f^+(x), f^-(x))$                     |

Table 1: WIPS expresses the other models by specifying $\lambda$ and $f_{\theta}$.

5.2 Interpreting WIPS as a Matrix Decomposition

Let $h_*$ be a general similarity function that is not limited to PD or CPD similarities. WIPS can be interpreted as the eigen-decomposition of the similarity matrix $H_*$ whose $(i,j)$-th entry is $h_*(x_i, x_j)$. Since $H_*$ is a symmetric real-valued matrix, it can be expressed as

$$H_* = U \Lambda U^\top,$$

where $U = (u_1, \ldots, u_n) \in \mathbb{R}^{n \times n}$ is the orthogonal matrix of unit eigen-vectors and and $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$ is the diagonal matrix of real eigenvalues $\lambda_k \in \mathbb{R}$. There will be negative $\lambda_k$’s when $h^*$ is a non-PD similarity. Let us reorder the eigenvalues so that $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$, and take the first $K$ eigen-vectors as $U_K = (u_1, \ldots, u_K) \in \mathbb{R}^{n \times K}$ and also $K$ eigenvalues as $\Lambda_K = \text{diag}(\lambda)$ with $\lambda = (\lambda_1, \ldots, \lambda_K)$. Now the similarity matrix is approximated as

$$H_* \approx U_K \Lambda_K U_K^\top.$$

We may define feature vectors $y_i \in \mathbb{R}^K$ for $x_i$, $i = 1, \ldots, n$ as $U_K^\top = (y_1, \ldots, y_n)$. This results in

$$h_*(x_i, x_j) \approx \langle y_i, y_j \rangle_{\lambda}$$

for all $1 \leq i < j \leq n$, and the accuracy improves in (3) as $K$ approaches $n$.

The representation learning with WIPS can be interpreted as a relaxed version of the matrix decomposition without any constraints such as the orthogonality of vectors. Instead, we substitute $y_i = f_{\theta}(x_i)$ in (3) and optimize the parameter vectors $\theta$ and $\lambda$ with an efficient algorithm such as SGD. The above interpretation gives an insight into how WIPS deals with general similarities; allowing negative $\lambda_k$ in WIPS is essential for non-PD similarities.

6. Experiments

6.1 Preliminary

Datasets We use the following networks and a text corpus.

- WebKB Hypertext Network\(^\dagger\) has 877 nodes and 1,480 links. Each node represents a hypertext. A link between nodes represents their hyperlink ignoring the direction.

\(^\dagger\) https://linqs.soe.ucsc.edu/data
Each node has a data vector of 1,409 dimensional bag-of-words. Each node also has semantic class label which is one of \{Student, Faculty, Staff, Course, Project\}, and university label which is one of \{Cornell, Texas, Washington, Wisconsin\}.

- **DBLP Co-authorship Network** (Prado et al., 2013) has 41,328 nodes and 210,320 links. Each node represents an author. A link between nodes represents any collaborations. Each node has a 33-dim. data vector that represents the number of publications in each of 29 conferences and journals, and topological properties of neighborhood.

- **WordNet Taxonomy Tree** (Nickel and Kiela, 2017) has 37,623 nodes and 312,885 links. Each node represents a word. A link between nodes represents a hyponymy-hypernym relation. 300 dimensional data vectors are prepared from Google’s pre-trained word embeddings\(^2\).

- **Text9 Wikipedia Corpus\(^3\)** consists of English Wikipedia articles containing about 123M tokens.

**Similarity models** We compare WIPS with baseline similarity models IPS, SIPS and IPDS (Okuno et al., 2018a,b) in addition to the negative Poincaré distance (Nickel and Kiela, 2017). Because most feature vectors obtained by Poincaré distance are close to the rim of Poincaré ball, we also consider a natural representation in hyperbolic space by transformation \( y_i \rightarrow 2y_i/(1 - \|y_i\|^2) \) for downstream tasks (denoted as Hyperbolic in Results). For computing feature vectors, we use a 3-layer fully connected neural network \( f_{\theta} : \mathbb{R}^p \rightarrow \mathbb{R}^K \) which consists of 2,000 hidden units with ReLU activation function. We focus only on the similarity models, because some experiments (Okuno et al., 2018a) showed that even the simplest IPS model with neural networks can outperform many existing feature learning methods, such as GraphSAGE (Hamilton et al., 2017). The neural network models are trained by an Adam optimizer with negative sampling approach (Mikolov et al., 2013; Tang et al., 2015) whose batch size is 64 and the number of negative sample is 5. The initial learning rate is grid searched over \{2e-4, 1e-3\}. The dimensionality ratio \( q/K \) of IPDS is grid searched over \{0.01, 0.25, 0.5, 0.75, 0.99\}. Instead, \( \lambda \) in WIPS is initialized randomly from the uniform distribution of range \((0, 1/K)\).

**Implementations** To make fair “apples to apples” comparisons, all similarity models are implemented with PyTorch framework upon the SIPS library\(^4\). We also made C implementation upon the word2vec program\(^5\). All our implementations will be publicly available.

### 6.2 Evaluation Tasks

To assess both the approximation ability of the proposed similarity model as well as the effectiveness of the learned feature vectors, we conduct the following tasks.

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- \(^2\) [https://code.google.com/archive/p/word2vec](https://code.google.com/archive/p/word2vec)
- \(^3\) [Extension of Text8 corpus, http://mattmahoney.net/dc/textdata](http://mattmahoney.net/dc/textdata)
- \(^4\) [https://github.com/kdrl/SIPS](https://github.com/kdrl/SIPS)
- \(^5\) [https://github.com/tmikolov/word2vec](https://github.com/tmikolov/word2vec)
Figure 2: Visualization of Hypertext Network. Two major semantic classes, Student (415 nodes) and Course (218 nodes), are plotted. 10 dimensional feature vectors are mapped to 2d space with T-SNE. The nodes are colored by its semantic labels (upper) for Student (navy) and Course (pink), and also university labels (lower) for Cornell (red), Texas (orange), Washington (green) and Wisconsin (blue). Both class labels are clearly identified with IPDS and WIPS, whereas they become obscure in the other embeddings.

**Reconstruction (Task 1)** Most settings are the same as those in Okuno et al. (2018b). To evaluate approximation capacity, we embed all nodes and predict all links, i.e., reconstruct the graph structure from the learned feature vectors. The maximum number of iterations for training is set to 100K. ROC-AUC of reconstruction error is evaluated at every 5K iterations and the best score is reported for each model.

**Link Prediction (Task 2)** To evaluate generalization error, we randomly split the nodes into train (64%), validation (16%) and test (20%) sets with their associated links. Models are trained on the sub-graph of train set and evaluated occasionally on validation set in iterations; the best evaluated model is selected. The maximum number of iterations and validation interval are 5K/100 for Hypertext Network, and they are 40K/2K for Co-authorship Network and Taxonomy Tree. Then, the trained models are evaluated by predicting links from unseen nodes of test set and ROC-AUC of the prediction error is computed. This is repeated for 10 times and the average score is reported for each model.

**Hypertext Classification (Task 3)** To see the effectiveness of learned feature vectors, we conduct hypertext classification with inductive setting. First, feature vectors of all nodes are computed by the models trained for Hypertext Network in Task 2, where $K$ is also optimized from $\{10, 50, 100\}$. Then, a logistic regression classifier is trained on the feature vectors of train set for predicting class labels. The classification accuracy is measured on test set. This is repeated for 10 times and the average score is reported for each model.

**Word Similarity (Task 4)** To see the quality of word embeddings from Text9 corpus, our similarity models are compared with four human annotated similarity scores: SimLex-999 (Hill et al., 2015), YP-130 (Yang and Powers, 2005), WS-Sim and WS-Rel (Agirre et al., 2009). The quality is evaluated by Spearman’s rank correlation. The models are trained by a SGD optimizer used in Mikolov et al. (2013) with 5 epochs and the learning rate is
Table 2: ROC-AUC for the reconstruction from fully observed data (Task 1) and the inductive link prediction of unseen nodes (Task 2). Boldface is the best, and underlines are 2nd and 3rd scores.

|         | IPS       | Poincaré  | Hyperbolic | SIPS     | IPDS     | WIPS     |
|---------|-----------|-----------|------------|----------|----------|----------|
| A       | 56.08     | 46.19     | 47.22      | 69.09    | 71.70    | **73.35**|
| B       | 91.59     | 30.17     | 93.12      | 93.81    | 93.81    | **96.31**|

Table 3: Classification accuracies on predicting (A) the semantic class label and (B) the university label (Task 3).

searched over \{0.01, 0.025\}. As additional baselines, we use Skip-gram (SG) (Mikolov et al., 2013) and Hyperbolic Skip-gram (HSG) (Leimeister and Wilson, 2018). Since SG learns two sets of embeddings, we also include SG with \(K/2\) dim. word vectors for fair comparisons. To compute similarities with SG, inner product and cosine similarity (denoted as SG and SG*) are used. Each model is trained 3 times and the average score is reported.

6.3 Results

We first verify that IPDS and WIPS are very similar in all the results. Since training of IPDS for each \(q\) takes about the same computation time as training of WIPS, the total computation time of WIPS is much shorter than IPDS. Looking at the reconstruction error in Table 2, the approximation capabilities of IPDS and WIPS are very high, followed by SIPS, Poincaré and IPS as expected from the theory. This tendency is clearly seen in the visualization of Fig. 2. Looking at the link prediction error in Table 2, the difference of models is less clear for generalization performance, but IPDS and WIPS still outperform
Table 4: Spearman’s $\rho$ on the word similarity task (Task 4).

the others. Table 3 shows the effectiveness of the feature vectors, where IPDS and WIPS have again the best or almost the best scores. As expected, the hyperbolic representation is much better than Poincaré ball model (Note: this does not apply to Table 2, because these two representations are in fact the same similarity model). Table 4 shows the quality of word embeddings. The new similarity models SIPS, IPDS and WIPS work well with similar performance to SG* (with twice the number of parameters), whereas IPS works poorly overall.

7. Conclusion

We proposed a new similarity model WIPS by introducing tunable element-wise weight in inner product. Allowing positive and negative weight values, it has been shown theoretically and experimentally that WIPS has the same approximation capability as IPDS, which has been proved to universally approximate general similarities. As future work, we may use WIPS as a building block of larger neural networks, or extend WIPS to tensor such as $\sum_{k=1}^{K} w_k y_k y_k'$ to represent relations of three (or more) feature vectors $y, y', y''$. This kind of consideration is obviously not new, but our work gives theoretical and practical insight to neural network architecture.

References

Eneko Agirre, Enrique Alfonseca, Keith Hall, Jana Kravalova, Marius Pasca, and Aitor Soroa. A Study on Similarity and Relatedness Using Distributional and WordNet-based Approaches. In Proc. of NAACL-HLT, pages 19–27, 2009. URL http://aclweb.org/anthology/N09-1003.

Aurélien Bellet, Amaury Habrard, and Marc Sebban. A survey on metric learning for feature vectors and structured data. arXiv:1306.6709, 2013.

A. Böttcher and P. Lancaster. Lectures on Operator Theory and Its Applications. Fields Institute monographs. Amer. Math. Soc., 1996. ISBN 9780821871867. URL https://books.google.co.jp/books?id=fTQQgKkqS8C.
Jane Bromley, Isabelle Guyon, Yann LeCun, Eduard Säckinger, and Roopak Shah. Signature verification using a “siamese” time delay neural network. In Advances in Neural Information Processing Systems 6, pages 737–744, 1994.

Gal Chechik, Uri Shalit, Varun Sharma, and Samy Bengio. An Online Algorithm for Large Scale Image Similarity Learning. In Advances in Neural Information Processing Systems 22, pages 306–314, 2009. URL http://papers.nips.cc/paper/3705-an-online-algorithm-for-large-scale-image-similarity-learning.pdf.

George Cybenko. Approximation by Superpositions of a Sigmoidal Function. Mathematics of Control, Signals, and Systems, 2(4):303–314, 1989.

Ken-Ichi Funahashi. On the approximate realization of continuous mappings by neural networks. Neural Networks, 2(3):183–192, 1989.

Jacob Goldberger, Geoffrey E Hinton, Sam T. Roweis, and Ruslan R Salakhutdinov. Neighbourhood components analysis. In Advances in Neural Information Processing Systems 17, pages 513–520, 2005. URL http://papers.nips.cc/paper/2566-neighbourhood-components-analysis.pdf.

Lev Goldfarb. A unified approach to pattern recognition. Pattern Recog., 17(5):575–582, 1984.

Werner Greub. Linear Algebra. Graduate texts in mathematics. Springer New York, NY, 1975. ISBN 978-1-4684-9446-4.

William L. Hamilton, Rex Ying, and Jure Leskovec. Inductive Representation Learning on Large Graphs. In Advances in Neural Information Processing Systems 30, pages 1024–1034, 2017.

Felix Hill, Roi Reichart, and Anna Korhonen. Simlex-999: Evaluating semantic models with genuine similarity estimation. Computational Linguistics, 41(4):665–695, December 2015. ISSN 0891-2017. doi: 10.1162/COLI_a_00237. URL http://dx.doi.org/10.1162/COLI_a_00237.

Brian Kulis et al. Metric learning: A survey. Foundations and Trends® in Machine Learning, 5(4):287–364, 2013.

Sun Yuan Kung. Kernel Methods and Machine Learning. Cambridge University Press, 2014.

Matthias Leimeister and Benjamin J. Wilson. Skip-gram word embeddings in hyperbolic space. arXiv:1809.01498, 2018.

Tomas Mikolov, Ilya Sutskever, Kai Chen, Greg Corrado, and Jeffrey Dean. Distributed Representations of Words and Phrases and Their Compositionality. In Advances in Neural Information Processing Systems 26, pages 3111–3119, 2013. URL http://dl.acm.org/citation.cfm?id=2999792.2999959.

Ha Quang Minh, Partha Niyogi, and Yuan Yao. Mercer’s Theorem, Feature Maps, and Smoothing. In International Conference on Computational Learning Theory (COLT), pages 154–168. Springer, 2006.
Maximillian Nickel and Douwe Kiela. Poincaré Embeddings for Learning Hierarchical Representations. In Advances in Neural Information Processing Systems 30, pages 6338–6347, 2017. URL http://papers.nips.cc/paper/7213-poincare-embeddings-for-learning-hierarchical-representations.pdf.

Maximillian Nickel and Douwe Kiela. Learning Continuous Hierarchies in the Lorentz Model of Hyperbolic Geometry. In Proc. of the 35th ICML, pages 3779–3788, 2018. URL http://proceedings.mlr.press/v80/nickel18a.html.

Dino Oglic and Thomas Gaertner. Learning in reproducing kernel Kreĭn spaces. In Proc. of the 35th ICML, pages 3859–3867, 2018. URL http://proceedings.mlr.press/v80/oglic18a.html.

Akifumi Okuno, Tetsuya Hada, and Hidetoshi Shimodaira. A probabilistic framework for multi-view feature learning with many-to-many associations via neural networks. In Proc. of the 35th ICML, pages 3885–3894, 2018a. URL http://proceedings.mlr.press/v80/okuno18a.html.

Akifumi Okuno, Geewook Kim, and Hidetoshi Shimodaira. Graph Embedding with Shifted Inner Product Similarity and Its Improved Approximation Capability. arXiv:1810.03463, 2018b. (to appear in AISTATS2019).

CS. Ong, X. Mary, S. Canu, and AJ. Smola. Learning with Non-Positive Kernels. In Proc. of the 21th ICML, pages 81–81, 2004.

Adriana Prado, Marc Plantevit, Céline Robardet, and Jean-François Boulicaut. Mining graph topological patterns: Finding covariations among vertex descriptors. IEEE Transactions on Knowledge and Data Engineering, 25(9):2090–2104, 2013.

Frank-Michael Schleif and Peter Tino. Indefinite proximity learning: A review. Neural Comput., 27(10):2039–2096, October 2015. ISSN 0899-7667. doi: 10.1162/NECO_a_00770. URL http://dx.doi.org/10.1162/NECO_a_00770.

Bernhard Schölkopf. The kernel trick for distances. In Advances in Neural Information Processing Systems 13, pages 301–307, 2001.

Jian Tang, Meng Qu, Mingzhe Wang, Ming Zhang, Jun Yan, and Qiaozhu Mei. LINE: Large-scale Information Network Embedding. In Proc. of the 24th WWW, pages 1067–1077, 2015. ISBN 978-1-4503-4349-3. doi: 10.1145/2736277.2741093. URL https://doi.org/10.1145/2736277.2741093.

Matus Telgarsky. Neural networks and rational functions. In Proceedings of the International Conference on Machine Learning (ICML), 06–11 Aug 2017. URL http://proceedings.mlr.press/v70/telgarsky17a.html.

Daixin Wang, Peng Cui, and Wenwu Zhu. Structural Deep Network Embedding. In Proc. of the 22nd ACM SIGKDD, pages 1225–1234, 2016. ISBN 978-1-4503-4232-2. doi: 10.1145/2939672.2939753. URL http://doi.acm.org/10.1145/2939672.2939753.
Hongteng Xu, Wenlin Wang, Wei Liu, and Lawrence Carin. Distilled Wasserstein Learning for Word Embedding and Topic Modeling. In Advances in Neural Information Processing Systems 31, pages 1723–1732, 2018. URL http://papers.nips.cc/paper/7443-distilled-wasserstein-learning-for-word-embedding-and-topic-modeling.

Shuicheng Yan, Dong Xu, Benyu Zhang, Hong-Jiang Zhang, Qiang Yang, and Stephen Lin. Graph embedding and extensions: A general framework for dimensionality reduction. IEEE Trans. Pattern Anal. Mach. Intell., 29(1):40–51, January 2007. ISSN 0162-8828. doi: 10.1109/TPAMI.2007.12. URL http://dx.doi.org/10.1109/TPAMI.2007.12.

Dongqiang Yang and David M. W. Powers. Measuring Semantic Similarity in the Taxonomy of WordNet. In Proc. of the 28th Australasian Conference on Computer Science - Volume 38, pages 315–322, 2005. ISBN 1-920-68220-1. URL http://dl.acm.org/citation.cfm?id=1082161.1082196.

Dmitry Yarotsky. Error bounds for approximations with deep ReLU networks. Neural Networks, 94:103–114, 2017.