Deep Kernel Supervised Hashing for Node Classification in Structural Networks

Jia-Nan Guo, Xian-Ling Mao, Shu-Yang Lin, Wei Wei and Heyan Huang
Beijing Institute of Technology, Beijing, China
Huazhong University of Science and Technology, China
{guojn, maoxl, hhy63}@bit.edu.cn
linshuyang2017@gmail.com
Wei@hust.edu.cn

Abstract

Node classification in structural networks has been proven to be useful in many real world applications. With the development of network embedding, the performance of node classification has been greatly improved. However, nearly all the existing network embedding based methods are hard to capture the actual category features of a node because of the linearly inseparable problem in low-dimensional space; meanwhile they cannot incorporate simultaneously network structure information and node label information into network embedding. To address the above problems, in this paper, we propose a novel Deep Kernel Supervised Hashing (DKSH) method to learn the hashing representations of nodes for node classification. Specifically, a deep multiple kernel learning is first proposed to map nodes into suitable Hilbert space to deal with linearly inseparable problem. Then, instead of only considering structural similarity between two nodes, a novel similarity matrix is designed to merge both network structure information and node label information. Supervised by the similarity matrix, the learned hashing representations of nodes simultaneously preserve the two kinds of information well from the learned Hilbert space. Extensive experiments show that the proposed method significantly outperforms the state-of-the-art baselines over three real world benchmark datasets.

1 Introduction

Networks are ubiquitous in the real world, and many real-world datasets take the form of networks such as social networks, citation networks, language networks and biological networks. Generally, networks can be divided into two categories: structural networks (Wang, Cui, and Zhu 2016) and attributed networks (Yang et al. 2018). Compared with attributed networks, structural networks are more widely used, which can be constructed by the most fundamental network structure information without using auxiliary information from node attributes.

In structural networks, node classification is one of the most typical learning tasks, which focuses on exploiting the node interactions to predict the missing labels of unlabeled nodes in a structural network. Many real world applications can be modeled as the node classification problem, such as profession identification (Tu et al. 2017) and persona classification (Kaul et al. 2020).

Generally speaking, existing node classification methods can be divided into two categories: traditional methods (Neville and Jensen 2000; Macskassy and Provost 2003; Yamaguchi, Faloutsos, and Kitagawa 2015) and network embedding based methods (Yang et al. 2015; Grover and Leskovec 2016; Dai et al. 2017, 2019). Compared with the traditional methods that directly infer posterior distribution of node labels from neighborhood information, network embedding based methods can achieve better performance by alleviating the curse of dimensionality for large-scale structural networks and avoiding cascading errors. However, nearly all the existing embedding based node classification methods in structural networks suffer from the following two problems: (1) They are hard to capture the actual category features hidden in highly nonlinear network structure, because of the linearly inseparable problem in low-dimensional space; (2) They are all unsupervised algorithms, and only preserve network structure information into network embedding without considering node label information.

To address the above problems, we propose a novel Deep Kernel Supervised Hashing, called DKSH, to learn node representations for node classification in structural networks. Specifically, a deep multiple kernel learning is first proposed to map nodes into suitable Hilbert space, which can deal with linearly inseparable problem of category features. Then, instead of only considering structural similarity and ignoring category similarity between two nodes, a novel similarity matrix is designed to merge both network structure information and node label information. Supervised by the similarity matrix, the learned hashing representations of nodes can simultaneously preserve the two kinds of information from the learned Hilbert space. Extensive experiments show that the proposed method significantly outperforms the state-of-the-art baselines over three real world benchmark datasets.

The main contributions of our work are summarized as follows:

• We design a deep kernel hashing to maps nodes into suitable Hilbert space, which can deal with linearly inseparable problem of category features so as to generate good-quality hashing representations of nodes for node classification.
• We define a novel similarity matrix in network embedding area to merge both network structure information and node label information. Supervised by the similarity matrix, the proposed method can incorporate simultaneously the two kinds of information into network embedding.

• Extensive experiments over three real world benchmark datasets show that the proposed method significantly outperforms the state-of-the-art baselines.

The rest of the paper is arranged as follows: In Section 2, we will first review the related work of node classification and kernel hashing. Then, the details of our DKSH will be presented in Section 3. Moreover, in Section 4, we will present the experimental results of node classification over three real world benchmark datasets. Finally, the conclusions will be given to summary our work in Section 5.

2 Related Work

2.1 Node Classification in Structural Networks

In this section, we discuss the recent trends and some state-of-the-art node classification methods in structural networks instead of attributed networks. Generally, existing node classification methods can be divided into two categories: traditional methods and embedding based methods.

Traditional methods [Neville and Jensen 2000; Mackay and Provost 2003; Yamaguchi, Faloutsos, and Kitagawa 2015] pose node classification as an inference in an undirected Markov network, and then use iterative approximate inference algorithms to directly compute the posterior distribution of labels given the network structure. For example, OMNI-Prop (Yamaguchi, Faloutsos, and Kitagawa 2015) assigns each node with the prior belief about its label and then updates the label using the evidence from its neighbors, i.e., if the most of neighbors have the same label, then the rest also have the same label. However, these methods have a high computational complexity, which suffer from the curse of dimensionality for large-scale structural networks; meanwhile they cannot avoid cascading errors.

Different from traditional methods, network embedding based methods learn a classifier from the learned low-dimensional node representations, which can achieve better performance by alleviating the curse of dimensionality for large-scale structural networks and avoiding cascading errors. Nowadays, network embedding based methods become the recent trend for node classification [Li and Pi 2019]. Essentially, this type of methods adopt following three steps [Cui et al. 2018]: (1) a network embedding algorithm, such as deep neural network [Perozzi, Al-Rfou, and Skiena 2014; Wang, Cui, and Zhu 2016] and matrix factorization [Ou et al. 2016; Wang et al. 2017b], is applied to learn low-dimensional node representations with preserving rich network structure information; (2) the nodes with known labels are used as the training set; (3) a classifier, such as support vector classifier [Dai et al. 2019] and logistic regression classifier [Grover and Leskovec 2016], is learned from the training set to perform node classification. The representative methods include DeepWalk [Perozzi, Al-Rfou, and Skiena 2014], node2vec [Grover and Leskovec 2016], SDNE [Wang, Cui, and Zhu 2016] and DWNS [Dai et al. 2019]. DeepWalk first adopts random walk to extract local structure information of a node into node representation and then use an one-vs-rest logistic regression for classification. node2vec adopts a flexible method for sampling node sequences to strike a balance between local and global structure information in network embedding process and then also use an one-vs-rest logistic regression classifier to classify. SDNE first adopts a deep autoencoder to simultaneously extract both the first-order and the second-order similarity into node representations and then uses a support vector classifier for classification. DWNS improves DeepWalk with generative adversarial networks (GANs) based regularization methods to generate better node representation and then also use a support vector classifier to classify. With these methods, the performance of node classification has been greatly improved.

The major problems of previous methods are that: (1) They are hard to capture the actual category features of a node because of the linearly inseparable problem; (2) They are unsupervised algorithms, and only preserve network structure information into network embedding without considering node labels. Among these methods, node2hash [Wang et al. 2018] is the closest to our DKSH, which also uses a kernel hashing method to obtain node representations from network information. However, their algorithm adopts a shallow kernel unsupervised hashing method [Shi et al. 2009], which is still suffer from the above two problems. In contrast, the proposed method adopts a deep kernel supervised hashing, which can address the above two problems well. Before introducing our deep kernel supervised hashing, the existing kernel hashing methods is briefly described in the next subsection.

2.2 Kernel Hashing

Kernel hashing is an useful method for nonlinear data, which maps original data into suitable Hilbert space and then learns hashing representations from this space. Generally, the existing kernel hashing methods can be categorized into single kernel hashing [He, Liu, and Chang 2010; Wang et al. 2018] and multiple kernel hashing [Liu, He, and Lang 2014; Zhu, Miao, and Tang 2018]. Compared with multiple kernel hashing, which is designed for multiple features data, single kernel hashing is the most fundamental method in kernel hashing. Thus, we take single kernel hashing as an example to introduce kernel hashing.

Single kernel hashing is an useful method to deal with classification tasks, which can learn hashing functions to map data from Hilbert space to hashing space. The formulation of hashing functions is:

\[ B_{mi} = h_m(X_i) = \text{sign}(V_m^T \varphi(X_i) - b_m) \]  

where \( h_m \) is m-th hashing code of data \( X_i \), \( \varphi \) is the function that maps original data to Hilbert space, \( V_m \) is a hyperplane vector in the Hilbert space and \( b_m \) is the threshold scalar. Note that, \( V_m \) is a linear weighted combination of \( R \) landmarks, which can be obtained by random choosing or clustering.
According to the definition of kernel matrix $K_{ij} = \varphi(X_i)^T \varphi(X_j)$, Equation (1) can be rewritten in a kernel form:

$$B_i = sign(W^T K_i - b)$$ (2)

where $W_{R\times M}$ is weighted matrix of landmarks, $K_i$ is i-th column of a designed kernel matrix $K_{R\times N}$. In this way, the formulation of hashing functions is obtained, which can be used to learn nonlinear features from many data modalities, especially image (He, Liu, and Chang 2010).

Nevertheless, both single kernel hashing and multiple kernel hashing adopt shallow kernel (Zhuang, Tsang, and Hoï 2011), which is often powerless to capture the actual features from highly nonlinear network data.

3 Deep Kernel Supervised Hashing

In this section, we first describe the problem formulation of node classification in structural networks, and then introduce the details of the proposed Deep Kernel Supervised Hashing (DKSH) method. The conceptual framework of DKSH is shown in Figure 1.

### 3.1 Problem Formulation

Formally, an undirected network is denoted as $G = (V, E, Y)$, where $V = \{v_i\}_{i=1}^{N}$ represents the set of $N$ nodes, $E = \{e_{ij}\}_{i,j=1}^{N}$ represents the set of edges between two nodes and $Y$ denotes the labels set. For $v_i$ and $v_j$ are linked by an edge, $e_{ij} = 1$. Otherwise, $e_{ij} = 0$. Network hashing embedding is to learn a set of hash functions $H = \{h_m\}_{m=1}^{M}$, which are used to map each node in $G$ into a low-dimension hashing representation $B_i \in \{-1, 1\}^M$. $M$ is the dimension of hashing representations.

Given the labeled node set $V_L$ and the unlabeled node set $V_N$, where each node $v_i \in V_L$ is associated with a label $y_i \in Y$ but not in another, our goal is to predict the missing labels of unlabeled nodes $V_N$ with the learned hashing representations $B$.

### 3.2 Preprocessing Algorithms

The algorithms of preprocessing is used to construct structure matrix by sampling network structure information and then similarity matrix by merging node labels and the structure matrix.

**Structure Matrix** In network embedding area, the random walk is one of the most popular and powerful network sampling methods, which reflects the rich network structure information of center node in $G$. Generally, the relationship extracted from random walks contains 0 and 1, where 0 is the relationship between unknown node pairs and 1 is the relationship between similar node pairs (Perozzi, Al-Rfou, and Skiena 2014). However, this type of relationship ignores the relative distance between center node and context nodes.
of it in window. Therefore, in this paper, we assign different weights to context nodes in window, according to their relative distance to the center node.

Initialising structure matrix $P = O$, where $O$ is zero matrix. For each similar node pairs $(v_i, v_j)$ in window $v$, where $v_i$ is the center node, $v_j$ is the context node of $v_i$ and $p$ is the window size, the recursive definition of $P$ is:

$$P'_{ij} = P_{ij} + \frac{p + 1 - \text{dis}(v_i, v_j)}{p}$$  \hfill (3)$$

where $\text{dis}(v_i, v_j)$ is to compute the relative distance between $v_i$ and $v_j$ in the window. Note that, $(p + 1 - \text{dis}(v_i, v_j))/p$ is the weight provided by $(v_i, v_j)$, which is negatively related to the relative distance. In this way, $P_{ij}$ can reflect simultaneously the relative distance and the co-occurrence frequency of $(v_i, v_j)$ in random walks. More details of constructing structure matrix is shown in Algorithm 1.

**Similarity Matrix** According to DeepWalk (Perozzi, Al-Rfou, and Skiena 2014), structure matrix reflects rich structure information, which can be treated as feature matrix. Thus, in order to simultaneously preserve network structure information and node label information, similarity matrix $S$ is defined as:

$$S_{ij} = \left\{ \begin{array}{ll} \exp\left(\frac{||P_i - P_j||}{\max \text{dis}(v_i, v_j)}\right), & y_j = y_i \\ 0, & \text{otherwise} \end{array} \right.$$  \hfill (4)$$

where, $P_i$ and $P_j$ are feature vectors of $v_i$ and $v_j$, $\max \text{dis}(v_i, v_j)$ is the max globally distance between all the feature vectors and $y_i$ is the label of node $v_i$.

### 3.3 Learning Deep Kernel Matrix

Learning a deep kernel matrix aims to map nodes into suitable Hilbert space, which detail the architecture and implementation of deep multiple kernel learning.

**Deep Multiple Kernel Learning** Multiple kernel learning (MKL) (Liu, He, and Lang 2014) is a widely used technique for kernel designing. Its principle consists in learning, for a given support vector classifier, the most suitable technique for kernel designing. Its principle consists in learning, for a given support vector classifier, the most suitable convex linear combination of standard elementary kernels. However, this kind of linear combination of kernels is a shallow way, which often cannot capture highly nonlinear features. In this way, deep multiple kernel learning (DKL) is proposed (Strobl and Visweswaran 2013; Jiu and Sahbi 2017). Interestingly, network structure information is just a highly nonlinear network information. Thus, in this section, we describe how to make DKL to fit network data.

Figure 2 shows the architecture of our DKL, which adopts a nonlinear multi-layered combination of multi-kernels. The recursive definition of our deep kernel is:

$$K^{(l)}_t = g_t\left(\sum_{t=1}^{T} \mu_{t}^{(l-1)} K^{(l-1)}_{t}\right)$$  \hfill (5)$$

where $g_t(\cdot)$ is the activation function for kernel matrix $K_t$ like $rbf(\cdot)$, which can map feature matrix (or kernel matrix) to kernel matrix. Moreover, we assume that the architecture of DKL has $L$ layers and each layer contains $T$ single kernel matrices, $l \in \{1, \cdots, L\}$, $t \in \{1, \cdots, T\}$. In this case, $K^{(l)}_t$ expresses the kernel matrix of $l$-th layer and $t$-th unit in this model. Besides, $K^{(l)}_t = g_t(P)$, where $P$ is the structure matrix of a structural network (see Algorithm 1), and the final output of the proposed DKL is $K = \sum_{t=1}^{T} (l) = \sum_{t=1}^{T} K^{(l)}_t$.

**Algorithm 2 Learning Deep Kernel Matrix**

**Require**: Initial network parameters $\mu = \frac{1}{L}$, structure matrix $P$, the number of nodes $N$.

**Ensure**: Optimal $\mu$, coefficients of SVM $\alpha$.

1. repeat
2. Fix $\mu$, compute output deep kernel $K$.
3. $\alpha$ is optimized by SVM solver.
4. Fix $\alpha$, compute the gradient $\nabla_{\mu}$ of $\text{fspan}_wrt K$.
5. Update weight $\mu$, according to $\nabla_{\mu}$, and keep $\mu \geq 0$.
6. until Convergence

**Implementation** In order to optimize the network parameters $\mu$ of the proposed DKL, we use the backward information from an one-vs-rest SVM classifier. The SVM classifier for network data is designed as $s_{g\text{in}}(\sum_{i=1}^{N} \alpha_i y_i K(v_i, v) + b)$, where $y_i$ is the label of node $v_i$. Generally, $\mu$ can be optimized by minimizing an objective function, which is a global hinge loss of the classifier like (Jiu and Sahbi 2017). However, in order to reduce the risk of over-fitting, we use span bound method to learn deep kernel (Liu, Liao, and Hou 2011). Under the assumption that the set of support vectors remains the same during the leave-one-out procedure, the span bound can be stated as:

$$\mathcal{L}((v_1, y_1), \cdots, (v_N, y_N)) \leq \sum_{i=1}^{N} \varphi(\alpha_i D_i^4 - 1)$$  \hfill (6)$$

where $\mathcal{L}$ is leave-one-out error, and $D_i$ is the distance between the point $\varphi(v_i)$ and the set $\Gamma_i = \{\sum_{j \neq i} \alpha_j \varphi(v_j) \mid \sum_{j \neq i} \lambda_j = 1\}$. Based on Equation (6), we can formulate the objective function of deep multiple kernel learning as minimize the upper bounds of
leave-one-out error:
\[
\min_{\mu, \alpha} T_{\text{span}} = \sum_{i=1}^{N} \varphi(\alpha_i D_i^2 - 1) \tag{7}
\]

Here, the objective function is optimized w.r.t two parameters: \(\mu\) and \(\alpha\). Alternating optimization strategy is adopted, i.e., we fix \(\mu\) to optimize \(\alpha\), and then vice-versa. At each iteration, when \(\mu\) is fixed, the deep kernel \(K\) is also fixed, \(\alpha\) can be auto-optimized using a SVM classifier \cite{Fan et al. 2008}. When \(\alpha\) fixed, \(\mu\) can be directly optimized by computing the gradient of Equation (7) \cite{Strobl and Visweswaran 2013}. The iterative procedure continues until convergence or when a maximum number of iterations is reached (see Algorithm 2).

### 3.4 Optimized Deep Kernel Hashing

The function of deep kernel hashing is used to learn the hashing representations of nodes from the learned Hilbert space. Note that, in the section of related work, we introduce the existing hashing kernel methods. However, both single kernel hashing and multiple kernel hashing are shallow kernel hashing methods, which are often powerless to learn a suitable Hilbert space for highly nonlinear network structure. In order to address this problem, we extend shallow kernel into the learned deep kernel. According to Equation (2) and Equation (4), the proposed deep kernel hashing functions can be written as:

\[
B_i = \text{sign}(W^T K_i - b) \tag{8}
\]

with

\[
K_{R \times N} = \sum_{t=1}^{T} \mu_t^{(L)} K_t^{(L)} R \times N
\]

where \(W_{R \times M}\) is weighted matrix of landmarks, \(K_i\) is \(i\)-th column of the learned deep kernel matrix \(K_{R \times N}\).

With the similarity matrix and the hashing functions, the form of similarity-distance product minimization \cite{Wang et al. 2017a} is adopted to design the following objective function for network hashing representation:

\[
\begin{align*}
    & \min_{W} \frac{1}{2} \sum_{i,j=1}^{N} S_{ij} \|B_i - B_j\|^2 + \lambda \sum_{m=1}^{M} \|V_m\|^2 \\
    & \text{s.t.} \quad N \sum_{i=1}^{N} B_i = 0 \\
    & \quad \frac{1}{N} \sum_{i=1}^{N} B_i B_i^T = I
\end{align*} \tag{9}
\]

where \(S\) is the similarity matrix. \(B_i\) is the hashing representation of \(v_i\) obtained from Equation (8), which has the same constraints. \(\sum_{m=1}^{M} \|V_m\|^2\) is utilized to a regularized term to control the smoothness of hyperplane vector \(V_m\). The constraint \(\sum_{i=1}^{N} B_i = 0\) is to make sure bit balance, i.e., 50% to be 1 and 50% to be -1. The constraint \(\frac{1}{N} \sum_{i=1}^{N} B_i B_i^T = I\) is to ensure bit uncorrelation. In this way, we can obtain compact hashing representations of nodes.

| Dataset | \(|V|\) | \(|E|\) | \(|Y|\) |
|---------|--------|--------|--------|
| Wiki    | 2,405  | 17,981 | 17     |
| Cora    | 2,708  | 5,429  | 7      |
| Citeseer| 3,312  | 4,732  | 6      |

Table 1: Statistics of Benchmark Datasets

Using Laplacian matrix \(L = \text{diag}(S \mathbf{1}) - S\), the objective function can be derived as:

\[
\begin{align*}
    & \min_{W} \frac{1}{2} \text{tr}(W^T (C + C^T) W) \\
    & \text{s.t.} \quad W^T GW = I
\end{align*} \tag{10}
\]

with

\[
\begin{align*}
    C &= K_{R \times N} L K_{R \times N}^T + \lambda K_{R \times R} \\
    G &= \frac{1}{N} K_{R \times N}(I - \frac{1}{N} \mathbf{1} \mathbf{1}^T) K_{R \times N}^T
\end{align*}
\]

Here, \(b = -\frac{1}{N}) W^T K_{R \times N} \mathbf{1}\), \(W_{R \times M}\) is weighted matrix of landmarks. Note that, the derivation follows \cite{He, Liu, and Chang 2010}.

**Implementation** For simpler implementation, Equation (10) can be further rewritten into an eigen vector problem:

\[
\begin{align*}
    & \min_{W} \text{tr}(\hat{W}^T \hat{C} \hat{W}) \\
    & \text{s.t.} \quad \hat{W}^T \hat{W} = I
\end{align*} \tag{11}
\]

with

\[
\begin{align*}
    \hat{C} &= \Lambda^{-\frac{1}{2}} T^T (C + C^T) T \Lambda^{-\frac{1}{2}} \\
    G &= T_0 \Lambda_0 T_0^T \\
    \hat{W} &= T \Lambda^{-\frac{1}{2}} \hat{W}
\end{align*}
\]

where \(\Lambda\) is a diagonal matrix consisting of \(M\) largest elements of \(\Lambda_0\), and \(T\) is the corresponding columns of \(T_0\). In this way, the solution of this eigen vector problem is matrix \(\hat{W}\), which is \(M\) eigen vectors of matrix \(\hat{C}\). Given \(\hat{W}\), \(\hat{W}\) can be directly obtained by \(\hat{W} = T_0 \Lambda_0 \hat{W}\). Based on \(\hat{W}\), we can get the hashing representations of \(v_i, i = 1, \cdots, N\), according to Equation (5).

Note that, after obtaining the hashing representations of nodes, an off-the-shelf classifier is trained to predict the missing labels of unlabeled nodes.

### 4 Experiments

In the previous section, the proposed method incorporates simultaneously network structure information and node label information into the hashing representations of nodes. In this section, extensive node classification experiments are conducted to verify that the proposed method can improve the performance of node classification in structural networks.
|                     | Wiki | Cora | Citeseer |
|---------------------|------|------|----------|
| % Labeled Nodes     | 80%  | 90%  | 80%      | 90%  | 80%  | 90%  |
| DeepWalk            | 68.37| 68.78| 79.35    | 79.23| 58.15| 59.11|
| Line                | 67.46| 67.63| 75.30    | 75.76| 55.93| 57.22|
| GraRep              | 65.18| 67.05| 80.89    | 80.74| 65.48| 56.39|
| node2vec            | 67.19| 68.73| 84.02    | 84.91| 68.11| 61.04|
| AIDW                | 66.58| 68.02| 84.11    | 83.69| 61.18| 62.84|
| Dwns                | 68.35| 69.32| 85.66    | 85.65| 63.05| 63.73|
| node2hash           | 55.18| 55.14| 79.11    | 79.56| 63.12| 64.72|
| DKSH-1              | 67.29| 77.67| 79.63    | 81.85| 64.60| 64.65|
| DKSH-2              | 68.13| **78.17**| 81.85 | 83.33| 64.90| 65.86|
| DKSH                | **70.83**| 77.08| 82.04    | **85.93**| 69.28| 68.58|

Table 2: Micro-accuracy (%) of Node Classification on Wiki, Cora and Citeseer

4.1 Experimental Setup

Datasets We conduct experiments on three real world benchmark datasets, which are popularly used in many previous works [Dai et al. 2017, 2019]. Cora and Citeseer are scientific paper citation networks constructed by [McCallum et al. 2000]. Wiki [Sen et al. 2008] is a network of Wikipedia pages. We regard these three networks as undirected structural networks, and do some preprocessing on the original datasets by deleting nodes with zero degree. The statistics of them is presented in Table 1.

Metric Following previous works [Dai et al. 2017, 2019], we employ the popularly used Micro-accuracy to evaluate the performance of node classification. Micro-accuracy measures the accuracy of the aggregated contributions of all classes, which is short for micro-averaged accuracy.

Baselines We compare our DKSH with the state-of-the-art baselines and its variants. For fair comparisons, all the baselines are structural network embedding methods without using node attributes information. Besides, among these baselines, node2hash is the only hashing representation method like our DKSH. The details of the baselines are as follows:

- **DeepWalk** [Perozzi, Al-Rfou, and Skiena 2014]: DeepWalk is an unsupervised method, which uses local structure information obtained from truncated random walks to learn low-dimensional feature representations of nodes.

- **Line** [Tang et al. 2015]: Line uses the breadth-first strategy to sample the inputs, based on node neighbors. The method preserves both the first-order and second-order similarity in network embedding process.

- **GraRep** [Cao, Lu, and Xu 2015]: GraRep applies SVD technique to different k-step probability transition matrix to learn node representations, and finally obtains global representations through concatenating all k-step representations.

- **node2vec** [Grover and Leskovec 2016]: node2vec differs from DeepWalk by proposing more flexible method for sampling node sequences to strike a balance between local and global structure information.

- **AIDW** [Dai et al. 2017]: AIDW is an inductive version of DeepWalk with GAN-based regularization methods. A prior distribution is imposed on node representations through adversarial learning to achieve a global smoothness in the distribution.

- **Dwns** [Dai et al. 2019]: Dwns is an improved AIDW, which introduces a succinct and effective regularization technique, namely adversarial training method, in network embedding process.

- **node2hash** [Wang et al. 2018]: node2hash uses the encoder-decoder framework, where the encoder is used to map the structural similarity of nodes into a feature space,
and the decoder is used to generate the hashing representations of nodes through a single kernel hashing.

Besides, we also include two additional baselines, namely DKSH-1 and DKSH-2, which respectively represent our DKSH model with 1-layer MKL and 2-layers MKL.

Parameter Settings For DKSH and its variants including DKSH-1 and DKSH-2, the window size $p$, walk length $l$, walks per nodes $γ$, number of kernel in each layer $T$, number of landmarks $R$ and regularization parameter $λ$ are respectively set to 10, 40, 80, 4, 256 and 0.0001. Different from DKSH-1 and DKSH-2, DKSH adopts a 3-layer DKL. Besides, the dimension of node representations are set to 128 for all methods, and the other parameters are set to be the default value for the baselines.

4.2 Comparison of Node Classification Performance

For node classification, we randomly sample a portion of labeled nodes, i.e., 80% and 90%, to train a support vector classifier in Liblinear [Fan et al. 2008]. Table 2 lists the results of node classification. Note that, some experimental results of the baselines follow DWNS (Dai et al. 2019), which has the same settings of the parameters and the classifier as in our work. From this table, it can be observed that:

- The proposed method DKSH consistently outperforms all the state-of-the-art baselines. As shown in Tables 2 Dwns produces better results than DeepWalk, LINE, GraRep, node2vec and AIDW. The proposed method can further achieve improvements over Dwns. More specifically, DKSH achieves the best classification accuracy on all three benchmark datasets across different training ratios, with only one exception on Cora with training ratio as 80%. Note that explanation of the exception is given in sensitivity of labeled ratio part in the next subsection.

- DKSH consistently outperforms DKSH-2, and DKSH-2 consistently outperforms DKSH-1 on three datasets across almost all training ratios, with only one exception on Wiki with training ratio as 90%. For example, DKSH consistently gives about 3% gain in Micro-accuracy over DKSH-2 on Citeseer, and DKSH-2 consistently gives about 1.5% gain in Micro-accuracy over DKSH-1 on Cora. These results demonstrate that it is easier to capture the actual category features of a node in a more suitable Hilbert space.

- It can significantly improve the performance of node classification by incorporating simultaneously network structure information and node label information into network embedding, instead of only network structure information. For example, compared with node2hash, DKSH-1 achieves more than 15% gain in Micro-accuracy on Wiki, more than 3% gain in Micro-accuracy on Wiki, and about 4% gain in Micro-accuracy on Citeseer across all training ratios.

- The hashing representation does not necessarily lead to accuracy loss. In fact, it may avoid over-fitting in this paper. For example, both DKSH and node2hash use hashing methods to learn compact hashing representations of nodes. The results show that DKSH is better than nearly all the non-hashing methods, and node2hash has a competitive performance compared with DeepWalk and node2vec.

4.3 Sensitivity Analysis

In this subsection, we analyze parameter sensitivity of the proposed model. Compared with other methods, DKSH has two exclusive parameters, the number of landmarks $R$ in the learned Hilbert space and labeled nodes rate in the process of learning node representations and classifier. Besides, the dimension of node representations $M$ is often necessary to evaluate model sensitivity in network embedding area. Thus, due to space constraint, in this subsection, we only examine how the number of landmarks $R$, labeled nodes rate and the dimension of node representations $M$ affect the performance of node classification over Wiki, Cora and Citeseer. Note that except for the parameter being tested, all the other parameters are set to default values.

Figure 3 (a) shows Micro-accuracy of our DKSH w.r.t. the number of landmarks $R$. When the dimension increases from $M$ to 1, 024, the Micro-accuracy relatively stable over the three benchmark datasets, which means our DKSH is not sensitive on the number of landmarks $R$. However, training time is positively correlated with $R$. Thus, we select an relatively small $R$, i.e., 256.

Figure 3 (b) shows Micro-accuracy of our DKSH w.r.t. labeled nodes rate. It can be easily noticed that the Micro-accuracy greatly increases when the labeled nodes rate varies from 40% to 90%, which is greatly sensitive. The reason why our DKSH is sensitive on labeled nodes rate is largely because our DKSH incorporates simultaneously network structure information and node label information into network embedding instead of only network structure information.

Figure 3 (c) shows Micro-accuracy of our DKSH w.r.t. the dimension of node representations $M$. DKSH achieves the best Micro-accuracy over the three benchmark datasets when $M = 128$. The reason why the Micro-accuracy over the three benchmark datasets improves first when $M$ varies from 16 to 128 is largely because more features are captured into higher dimension of node representation. However, when the dimension further increases to 256, the linear SVM classifier is powerless to classify these high-dimensional node representations.

5 Conclusions

In this paper, we propose a novel Deep Kernel Supervised Hashing (DKSH) method to learn the hashing representations of nodes for node classification in structural networks. In DKSH, we designed a deep kernel hashing to mapping highly non-linear network structure information into suitable Hilbert space to deal with linearly inseparable problem, and define a novel similarity to incorporate simultaneously network structure information and node label information into network embedding. The experimental results demonstrate the superior usefulness of the proposed method in node classification.
References

Cao, S.; Lu, W.; and Xu, Q. 2015. Grarep: Learning graph representations with global structural information. In Proceedings of the 24th ACM international on conference on information and knowledge management, 891–900.

Cui, P.; Wang, X.; Pei, J.; and Zhu, W. 2018. A survey on network embedding. IEEE Transactions on Knowledge and Data Engineering 31(5): 833–852.

Dai, Q.; Li, Q.; Tang, J.; and Wang, D. 2017. Adversarial network embedding. arXiv preprint arXiv:1711.07838.

Dai, Q.; Shen, X.; Zhang, L.; Li, Q.; and Wang, D. 2019. Adversarial training methods for network embedding. In The World Wide Web Conference, 329–339.

Fan, R.-E.; Chang, K.-W.; Hsieh, C.-J.; Wang, X.-R.; and Lin, C.-J. 2008. LIBLINEAR: A library for large linear classification. Journal of machine learning research 9(Aug): 1871–1874.

Grover, A.; and Leskovec, J. 2016. node2vec: Scalable feature learning for networks. In Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining, 855–864.

He, J.; Liu, W.; and Chang, S.-F. 2010. Scalable similarity search with optimized kernel hashing. In Proceedings of the 16th ACM SIGKDD international conference on Knowledge discovery and data mining, 1129–1138. ACM.

Jiu, M.; and Sahbi, H. 2017. Nonlinear deep kernel learning for image annotation. IEEE Transactions on Image Processing 26(4): 1820–1832.

Kaul, A.; Mittal, V.; Chaudhary, M.; and Arora, A. 2020. Persona Classification of Celebrity Twitter Users. In Digital and Social Media Marketing, 109–125. Springer.

Li, B.; and Pi, D. 2019. Learning deep neural networks for node classification. Expert Systems with Applications 137: 324–334.

Liu, X.; He, J.; and Lang, B. 2014. Multiple feature kernel hashing for large-scale visual search. Pattern Recognition 47(2): 748–757.

Liu, Y.; Liao, S.; and Hou, Y. 2011. Learning kernels with upper bounds of leave-one-out error. In Proceedings of the 20th ACM international conference on Information and knowledge management, 2205–2208.

Macskassy, S. A.; and Provost, F. 2003. A simple relational classifier. Technical report, NEW YORK UNIV NY STERN SCHOOL OF BUSINESS.

McCallum, A. K.; Nigam, K.; Rennie, J.; and Seymore, K. 2000. Automating the construction of internet portals with machine learning. Information Retrieval 3(2): 127–163.

Neville, J.; and Jensen, D. 2000. Iterative classification in relational data. In Proc. AAAI-2000 workshop on learning statistical models from relational data, 13–20.

Ou, M.; Cui, P.; Pei, J.; Zhang, Z.; and Zhu, W. 2016. Asymmetric transitivity preserving graph embedding. In Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining, 1105–1114. ACM.

Perozzi, B.; Al-Rfou, R.; and Skiena, S. 2014. Deepwalk: Online learning of social representations. In Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining, 701–710. ACM.

Sen, P.; Namata, G.; Bilgic, M.; Getoor, L.; Galligher, B.; and Eliassi-Rad, T. 2008. Collective classification in network data. AI magazine 29(3): 93.

Shi, Q.; Petterson, J.; Dror, G.; Langford, J.; Smola, A.; Strehl, A.; and Vishwanathan, S. 2009. Hash kernels. In Artificial intelligence and statistics, 496–503.

Strobl, E. V.; and Visweswaran, S. 2013. Deep multiple kernel learning. In 2013 12th International Conference on Machine Learning and Applications, volume 1, 414–417. IEEE.

Tang, J.; Qu, M.; Wang, M.; Zhang, M.; Yan, J.; and Mei, Q. 2015. Line: Large-scale information network embedding. In Proceedings of the 24th international conference on world wide web, 1067–1077.

Tu, C.; Liu, Z.; Luan, H.; and Sun, M. 2017. PRISM: Profession identification in social media. ACM Transactions on Intelligent Systems and Technology (TIST) 8(6): 1–16.

Wang, D.; Cui, P.; and Zhu, W. 2016. Structural deep network embedding. In Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining, 1225–1234.

Wang, J.; Zhang, T.; Sebe, N.; Shen, H. T.; et al. 2017a. A survey on learning to hash. IEEE transactions on pattern analysis and machine intelligence 39(4): 769–790.

Wang, Q.; Wang, S.; Gong, M.; and Wu, Y. 2018. Feature Hashing for Network Representation Learning. In IJCAI, 2812–2818.

Wang, X.; Cui, P.; Wang, J.; Pei, J.; Zhu, W.; and Yang, S. 2017b. Community preserving network embedding. In AAAI, volume 17, 203–209.

Yamaguchi, Y.; Faloutsos, C.; and Kitagawa, H. 2015. Omni-prop: Seamless node classification on arbitrary label correlation. In Twenty-Ninth AAAI Conference on Artificial Intelligence. Citeseer.

Yang, H.; Pan, S.; Zhang, P.; Chen, L.; Lian, D.; and Zhang, C. 2018. Binarized attributed network embedding. In 2018 IEEE International Conference on Data Mining (ICDM), 1476–1481. IEEE.

Zhu, M.; Miao, H.; and Tang, J. 2018. Multi-Kernel Supervised Hashing with Graph Regularization for Cross-Modal Retrieval. In 2018 24th International Conference on Pattern Recognition (ICPR), 2717–2722. IEEE.

Zhuang, J.; Tsang, I. W.; and Hoi, S. C. 2011. Two-layer multiple kernel learning. In Proceedings of the Fourteenth International Conference on Artificial Intelligence and Statistics, 909–917.