OCGNN: One-class Classification with Graph Neural Networks

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Abstract

Nowadays, graph-structured data are increasingly used to model complex systems. Meanwhile, detecting anomalies from graph has become a vital research problem of pressing societal concerns. Anomaly detection is an unsupervised learning task of identifying rare data that differ from the majority. As one of the dominant anomaly detection algorithms, One Class Support Vector Machine has been widely used to detect outliers. However, those traditional anomaly detection methods lost their effectiveness in graph data. Since traditional anomaly detection methods are stable, robust and easy to use, it is vitally important to generalize them to graph data. In this work, we propose One Class Graph Neural Network (OCGNN), a one-class classification framework for graph anomaly detection. OCGNN is designed to combine the powerful representation ability of Graph Neural Networks along with the classical one-class objective. Compared with other baselines, OCGNN achieves significant improvements in extensive experiments.

1 Introduction

Nowadays, graph-structured data are increasingly used to model complex systems, ranging from social media networks [Peng et al., 2019], traffic networks [Yu et al., 2018], financial networks [Weber et al., 2018] to protein interaction networks [Fout et al., 2017]. A graph consists a pair $G = (V,E)$, where $V$ is a set of nodes, and $E$ is a set of edges. By the introduction of edges between data instances, graph can provide a powerful tool for effectively capture long-range correlations between them. Meanwhile, detecting anomalies from graph has become a vital research problem of pressing societal concerns [Akoglu et al., 2015]. Firstly, anomalous graph data can disrupt the performance of machine learning algorithms and bring serious consequences. Secondly, graph anomaly detection (GAD) has significant implications in many security-related domains, such as discovering suspicious financial transactions, monitoring traffic jams and unveiling malicious users in social networks.

Anomaly detection (or outlier detection) can be regarded as the task of identifying rare data items that differ from the majority of the data. As one of the dominant anomaly detection algorithms, hypersphere learning approaches, mainly involving One Class Support Vector Machine (OCSVM) [Schölkopf et al., 2001] and Support Vector Data Description (SVDD) [Tax and Duin, 2004], typically try to define a boundary around the given normal class data. Afterwards, whether the unknown data point is anomalous is determined by their location with respect to the boundary.

Although those traditional anomaly detection methods have been applied in diverse domains [Pimentel et al., 2014], they lost their effectiveness in graph data [Zhang et al., 2018]. Traditional machine learning methods can only handle Euclidean data (e.g., images, audio and texts and tabular data). In this case, data objects are treated as points lying in a multi-dimensional Euclidean space independently. But nodes in graph may exhibit inter-dependencies, which means they are inherently related to one another. Graph embedding methods, such as DeepWalk [Perozzi et al., 2014], can be used to map node relationship information into a fixed-length feature vector. Afterwards, traditional anomaly detection methods can be trained from that vector. However, these two-stage methods are decoupled in the sense that the graph embedding learning is task agnostic and not customized for GAD, which has an indirect contribution to detecting anomalous nodes.

In addition to traditional Euclidean data anomaly detection techniques, previous graph theory based GAD works [Akoglu et al., 2015] have achieved empirical success. These GAD works usually adopt graph matrix factorization to locate the anomaly subgraph or find the target community at first and then detect outlier in a certain subspace. However, there are several challenges existing: (i) Data nonlinearity. The nodal feature and interactions among nodes are highly non-linear while most of GAD methods rely on linear mechanisms. (ii) Computational complexity. In the Era of data deluge, real graphs can easily have millions of nodes and edges. The Computational overhead of classical GAD methods discourages their applicability to large-scale graphs. (iii) More importantly, researchers and developers are proficient in simple off-the-shelf Euclidean anomaly detection techniques. Graph theory based GAD methods increase their understanding and deployment costs, which greatly limits the development of graph mining community.

To the best of our knowledge, little effort has been made to address those problems. There needs to be an end-
to-end, easy-to-understand and powerful GAD technology. In this work, We propose One Class Graph Neural Network (OCGNN), a hypersphere learning framework for GAD. Graph Neural Networks (GNNs), a significant stride of graph mining domain, is a promising method to operate directly on non-Euclidean data [Xu et al., 2019]. GNNs is essentially a message passing (or neighborhood node aggregation) scheme, where each node aggregates feature information of its neighbors to compute its new feature vector. After multiple iterations of information aggregation, the feature vector of a node will captures the structural information among the node’s neighborhood. Even though GNNs have achieved outstanding performance in many graph mining tasks, it remains unclear how to exploit their potentiality for GAD problem.

OCGNN is designed to combine the powerful representation ability of GNNs along with the classical hypersphere learning objective. Because the topology information on the graph is automatically extracted by the GNNs, People can handle GAD problem without complicated graph theory. Furthermore, OCGNN is end-to-end because the node representation learned by OCGNN is highly related to the GAD task, which means the embeddings learned from OCGNN is more friendly to the downstream anomaly detection tasks than DeepWalk. By aggregating the neighborhood information, OCGNN compute the node embedding of each observable node. Whereas, hypersphere-learning objective aims at minimizing the volume of a hypersphere that encloses those embedding vectors [Ruff et al., 2018]. An anomalous node is defined by whether the location of its embedding is out of the hypersphere. Since OCGNN can extract the characterization from a dataset and learn node embeddings without label information, OCGNN can also be regarded as an unsupervised node embedding method designed for GAD.

Specifically, our contributions are listed as follows.

1. We derive a novel end-to-end OCGNN framework, which aims at applying the powerful representation ability of GNNs into graph anomaly detection problems. To the best of our knowledge, this is one of the first GNN-based work to address this problem.

2. A OCOSVM-like loss function is proposed to drive the training of the GNN, thus OCGNN is a natural extension of OCOSVM in the field of graph data. People can use OCGNN to handle GAD problem without any complicated graph theory, which will greatly strengthen the development of graph mining techniques.

3. OCGNN framework can be formed by any suitable paradigm of GNN layer. In our experiments, we use three popular GNN layers and three widely-used public graph datasets to illustrate the superiority of OCGNN.

### Table 1: Commonly Used Notations.

| Notations | Descriptions |
|-----------|--------------|
| $V = \{v_1, \ldots, v_N\}$ | The set of N nodes in a graph |
| $V_{tr} \subseteq V$, $|V_{tr}| = K$ | The set of K training nodes |
| $X \in \mathbb{R}^{N \times D}$ | Node feature matrix |
| $A \in \mathbb{R}^{N \times N}$ | Adjacency matrix |
| $g (X, A; W)$ | A graph neural network |
| $Z = g (X, A; W)$ | Node embedding matrix, $Z \in \mathbb{R}^{N \times F}$ |
| $[\cdot]^+ = \max(0, \cdot)$ | Non-negative operator |

### Definition 1. Attributed graph: An attributed graph is $G = (V, E, X)$, where $V = \{v_1, \ldots, v_N\}$ is the set of $N = |V|$ nodes, $E \subseteq V \times V$ is the set of $M = |E|$ edges between nodes and $X \in \mathbb{R}^{N \times D}$ denotes features for nodes. The structure of graph can be represented by an adjacency matrix $A \in \mathbb{R}^{N \times N}$, where $A_{i,j} = 1$ if there is an edge between node $v_i$ and $v_j$, otherwise $A_{i,j} = 0$.

### Definition 2. Anomaly detection: Given the anomaly-free training dataset $\{x_i, i = 1, \ldots, K\}$, the model is trained to describe the boundary of normal data, and then model produces the anomaly score $S(x_u)$ for an unseen data point $x_u$. A data point with high anomaly score is defined as an outlier.

### Definition 3. Node-wise graph anomaly detection: Given a graph, all nodes $X$, edges $A$ and only a part of nodes labels are available for training. Afterwards, the prediction of remaining unlabeled nodes is computed by the trained model. In training phase, all label-provided nodes belong to one class (normal), while remaining testing nodes belong to two classes (normal and abnormal).

### 2.2 Hypersphere Learning

Hypersphere learning is originally proposed in SVDD [Tax and Duin, 2004], which aims at learning an compact hypersphere boundary to cover all training data and detecting which (new) objects resemble this training set. In the application of anomaly detection, the training data are all normal, so hypersphere learning model can obtain a description boundary of normal data, then outliers can be precluded.

Let $X \subseteq \mathbb{R}^d$ be the data space, $\phi_k : \mathcal{X} \to \mathcal{F}_k$ be a mapping function from data space $\mathcal{X}$ to reproducing kernel Hilbert space $\mathcal{F}_k$, where $k : \mathcal{X} \times \mathcal{X} \to [0, \infty)$ is a positive-definite kernel function. The objective of SVDD is to describe the smallest hypersphere, in feature space $\mathcal{F}_k$, with center $c \in \mathcal{F}_k$ and radius $r > 0$ that encloses the majority of the training data. Given a training dataset $\mathcal{X}_K = \{x_i \in \mathcal{X}, i = 1, \ldots, K\}$, SVDD solves the primal problem:

\[
\min_{r,c} r^2 + \frac{1}{K} \sum_{i=1}^{K} \xi_i
\]

\[
s.t. \| \phi_k (x_i) - c \|_{\mathcal{F}_k}^2 \leq r^2 + \xi_i, \xi_i \geq 0, \forall i
\]

where $\xi_i$ are non-negative slack variables to allow the contamination of outliers in the training dataset. The data points $\phi_k (x_i) \in \mathcal{F}_k$ are not strictly inside the hypersphere, but the data located too away from the boundary should be penalized. The hyperparameter $\beta \in (0, 1]$ controls the trade-off between...
the sphere volume and the penalties. After minimizing Eq. 1, the center \( c \) and radius \( r \) can be obtained, while \( \xi \) is not a learnable parameter. Data point \( x_i \) that falls outside the hypersphere, i.e., \( \| \phi_k(x_i) - c \|^2 \geq r^2 \), is defined as outlier.

3 One Class Graph Neural Network

In this section, we introduce our OCGNN with OCGNN objective, basic bone, and optimization strategy, respectively.

3.1 The OCGNN Objective

With classical hyperspherical learning objective, SVDD model build a minimum volume hypersphere estimation of given data. However, our OCGNN learn useful node representations together with the hypersphere learning objective. To achieve this goal, we introduce GNN that is jointly trained to learning node embeddings by considering both node attributes and relationships and keep the embeddings into a minimum hypersphere.

GNNs consider both the node attributes \( X \in \mathcal{R}^{N \times D} \) and the adjacency matrix \( A \in \mathcal{R}^{N \times N} \) when learning the node embedding vectors \( Z \in \mathcal{R}^{N \times F} \). We use \( g(X, A; \mathcal{W}) \) to represent a GNN with layer-wise trainable weight set \( \mathcal{W} = \{ W^{(1)}, \ldots, W^{(L)} \} \) where \( L \in \mathcal{N} \) is the number of hidden layers. For a specific \( l \)th layer, the forward propagation rule of GNN can be summarized as:

\[
H^{(l+1)} = g\left(H^{(l)}, A; W^{(l)}\right), \tag{2}
\]

where \( H^{(l)} \) is the input for the \( l \)th GNN layer and \( H^{(l+1)} \) is the output after this layer. Note that the node attributes \( X \) is the input of the first layer, which equals to \( H^{(0)} \). The embedding matrix of the nodes \( Z \) is the final output \( H^{(L)} \). Thanks to the powerful GNN node embedding, it helps the performance improvement of down-stream tasks, such as node-level and graph-level classification and link prediction.

The aim of OCGNN is to jointly learn the net parameters \( \mathcal{W} \) and minimize the volume of the data description hypersphere which is characterized by a radius \( r \in \mathcal{R}^+ \) and a center \( c \in \mathcal{R}^F \). Given a graph defined by \( (X, A) \) and the set of \( K \) training nodes \( V_{tr} \subseteq V \), where \( K = \{|i: v_i \in V_{tr}\}\}, \) the objective of OCGNN is set as:

\[
\mathcal{L}(r, \mathcal{W}) = \frac{1}{\beta K} \sum_{v_i \in V_{tr}} \left(\|g(X, A; \mathcal{W})_{v_i} - c\|^2 - r^2\right)^+ + r^2 + \frac{\lambda}{2} \sum_{l=1}^{L} \|W^{(l)}\|^2 \tag{3}
\]

In the forward propagation, OCGNN receives all nodes and edges information in a graph and then output a node embedding matrix \( Z = g(X, A; \mathcal{W}), Z \in \mathcal{R}^{N \times F} \). However, only \( K \) node embeddings \( \{z_{v_i}, v_i \in V_{tr}\} \) are used in the loss function computation. The first term of Eq.3 is a penalty for node embeddings lying out of the hypersphere, i.e., if the distance between an embedding vector and the center \( c \) is greater than the radius \( r \). The hyperparameter \( \beta \in (0, 1] \) controls the trade-off between the sphere volume and the penalties (we will discuss it later). As in classical SVDD, the second term, minimizing \( r^2 \), is to minimize the volume of sphere. The last term is the weight decay regularizer on the OCGNN network parameters \( \mathcal{W} \) with a hyperparameter \( \lambda > 0 \).

The OCGNN objective lets the network learn to map the node embeddings that are closed the center \( c \) of the sphere. Since the training nodes are all normal, OCGNN will extract the common factors of the given nodes. As a result, the description boundary of normal nodes can be obtained and the anomalous nodes can be detected.

For a node \( v_i \) in the given graph, its anomaly score \( S(v_i) \) can be defined by the location of the embedding respect to the sphere: \( S(v_i) = \|g(X, A; \mathcal{W})_{v_i} - c\|^2 - r^2 \). If \( S(v_i) > 0 \), the node \( v_i \) is anomalous, otherwise it is a normal node. Note that the network parameters \( \mathcal{W}^* \) and the learned radius \( r^* \) can characterize a trained OCGNN model. The memory complexity of OCGNN is very low because no data need be stored for model prediction.

To explain the role of \( \beta \), we define \( \xi = \frac{\lambda}{2} \sum_{l=1}^{L} \|W^{(l)}\|^2 \) and \( d_{v_i} = \|g(X, A; \mathcal{W})_{v_i} - c\|^2 \), where \( i = 1, \ldots, K \). Assuming that there is a node subset \( V_o \subset V_{tr} \) whose nodes are mapped outside of the sphere by OCGNN, consisting \( K_o = \{|i: d_{v_i} > r^2, v_i \in V_{tr}\}\} \). Thus the OCGNN optimization problem for \( r \) can be written as:

\[
\operatorname{argmin}_{r} r^2 + \frac{1}{\beta K} \sum_{v_i \in V_o} (d_{v_i} - r^2) + \xi = \operatorname{argmin}_{r} \left(1 - \frac{K_o}{K}\right)r^2 + \frac{1}{\beta K} \sum_{v_i \in V_o} d_{v_i} + \xi \tag{4}
\]

So since the second and third term of Eq.4 is non-negative, radius \( r \) is decreased as long as \( K_o \leq \beta K \). That is, \( \frac{K_o}{K} \leq \beta \) must satisfy the optimum, which means \( \beta \) is an upper bound on the fraction of anomalous training nodes. The optimal radius \( r^* \) is determined by the largest \( K_o \) that satisfies the inequality, because if the inequality is not satisfied, the model cannot continue to minimize \( r \). Hence we also have \( \frac{K_o}{K} > \beta \). \( \beta \) is a lower bound on the fraction of samples being outside of the hypersphere. \( \beta \) allows some nodes to be mapped out of the sphere, otherwise, in order to enclose all training nodes, the radius \( r \) will be so large that OCGNN will fail to detect outliers.

3.2 The Bone of OCGNN

Our OCGNN is a GNN-based GAD framework, so its bone can be formed by any suitable GNN layer, such as Graph Convolutional network (GCN) [Kipf and Welling, 2017], Graph Attention Network (GAT) [Velickovic et al., 2018] and GraphSAGE [Hamilton et al., 2017]. In this section, we use GCN as an example to illustrate how OCGNN learns the node representation. GCN is one of the best paradigms of graph learning model. It is a multi-layer GNN model which expands the Eq. 2 as follows:

\[
g\left(H^{(l)}, A; W^{(l)}\right) = \sigma \left(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)}\right), \tag{5}
\]
Input: Attributed Graph $G = (V, E, X)$, normal nodes set $V_{tr}$, Slack parameter $\beta \in [0, 1]$, weight decay $\lambda > 0$
Output: Weights $W$, center $c \in \mathbb{R}^K$ and radius $r \in \mathbb{R}^+$

1. Initialize $W$ using Glorot uniform initialization.
2. Initialize $r = 0$, $c = \frac{1}{K} \sum_{v \in V_{tr}} g(X, A; W)v_i$.
3. while epoch < max-epoch do
4. \hspace{1em} $d_{tr} = \|g(X, A; W)v_{tr} - c\|^2$, $d_{tr} \in \mathbb{R}^n$.
5. \hspace{1em} $L = \frac{1}{2r^2} \sum_{v \in V_{tr}} (d_{tr} - r^2)^+ + r^2 + \lambda \sum_{i=1}^n \|W^{(l)}\|^2$.
6. \hspace{1em} Update $W$ by its stochastic gradient $\nabla_W L$.
7. \hspace{1em} if epoch mod $\phi = 0$ then
8. \hspace{2em} Update $r$ using $(1 - \beta) \times 100\%$ percentile of $d_{tr}$.
9. \hspace{1em} end if
10. end while
11. return $W$, $c$ and $r$

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
Datasets & Nodes & Edges & Feat. & Train/Val/Test nodes \\
\hline
Cora & 2708 & 5429 & 1433 & 490/246/410 \\
Citeseer & 3327 & 4732 & 3703 & 420/210/352 \\
Pubmed & 19717 & 44338 & 500 & 4725/2364/3936 \\
\hline
\end{tabular}
\caption{Summary of the datasets used in our experiments.}
\end{table}

4 Experiments

In this section, we introduce the detailed experimental setup and results, including datasets, baselines, network structure, hyperparameters selection and performance analysis. Source code is implemented using PyTorch and Deep Graph Library [Wang et al., 2019], which will be released at a Github repository.

4.1 Datasets

We use three publicly available and broadly used citation network datasets to evaluate our OCGNN model. All the dataset characteristics are summarized in Table 2. The publications and citation links are represented as nodes and edges, respectively. The node feature of each publication is described by a sparse bag-of-words feature vector computed from a dictionary. The Cora dataset has 7 categories of machine learning papers: Case Based, Genetic Algorithms, Neural Networks, Probabilistic Methods, Reinforcement Learning, Rule Learning, Theory; The Citeseer dataset consists of 6 paper classes: Agents, AI, DB, IR, ML, HCI; Each publication in the Pubmed dataset is classified into one of three classes (“Diabetes Mellitus, Experimental”, “Diabetes Mellitus Type 1”, “Diabetes Mellitus Type 2”). [Sen et al., 2008] provides more details about these datasets. The node anomaly detection datasets used in this paper is generated from the plain node classification datasets by random splitting. Note that different random seeds will generate different datasets. For each dataset, we choose the classes type set in bold as the normal class, and the remaining classes are used to represent anomalous class. All the nodes in the train set pertain to the normal class, while, for validation or test set, half of the nodes are normal and the other half are sampled from anomalous class. For all the methods we use in this paper, the hyperparameters are tuned in the validation set, then the performances are evaluated in the test set.

4.2 Baselines

Followed by [Velickovic et al., 2019], we compared our end-to-end OCGNN method with the twelve two-stage methods which are the combination of graph embedding methods and traditional anomaly detection algorithms. The first stage method, graph embedding, is used to learn and map the graph structure information into a fixed length embedding vector. For the second stage, traditional Euclidean anomaly detection methods can be trained by the embedding vector and node feature vector. We use DeepWalk [ Perozzi et al., 2014] to learn a 128-dimensional embedding as the first stage method with the same hyperparameter reported in [Kipf and Welling, 2017]. We choose four popular anomaly detection methods as the second stage. (i) OCSVM is our source method which
we have described above. It has an important parameter $\beta$, which is chosen as the same as our OCGNN model. (ii) Isolation Forest (IF) [Liu et al., 2008] is an efficient method of detecting anomaly data in high-dimensional datasets. IF recursively and randomly splits the data feature and stores this in a forest data structure. Outliers are defined as the data who have shorter path in the tree because it means the data need a smaller number of splittings from other majority data. (iii) PCA [Olive, 2017] and AutoEncoder [Thompson et al., 2002], two popular reconstruction-based approaches, assume that anomalies are incompressible and thus cannot be effectively reconstructed from low-dimensional projections.

### 4.3 OCGNN Setup

Our OCGNN is a GNN framework for GAD, and its bone can be formed by any suitable GNN layer. To evaluate the performance of OCGNN, we use three popular GNN layer paradigms, GCN [Kipf and Welling, 2017], GAT [Velickovic et al., 2018] and GraphSAGE [Hamilton et al., 2017], whose model configurations are almost same. To better demonstrate the true performance of the OCGNN framework, we use the same hyperparameters for training in all datasets and OCGNN models. The penalty parameter $\beta$ is set as 0.1. The OCGNN model is initialized with Glorot uniform weight initialization [Glorot and Bengio, 2010] and optimized by the AdamW [Loshchilov and Hutter, 2019] SGD optimizer with a learning rate of 0.001. During training, we apply weight decay regularization with $\lambda = 0.0005$. We trained each OCGNN model using an early stopping strategy on both the OCGNN loss (Eq. 3) and AUC score on the validation set, with a maximum of 5000 epochs and a patience of 100 epochs. For Cora and Citeseer datasets, we apply a two-hidden-layers GNN model with the hidden size of 64. For pubmed dataset, we use a single-hidden-layers GNN model with hidden size of 128. For each individual OCGNN model, the final dimension of output layer (the dimension of node embedding) is always the half of the hidden size. After each GNN layer, the dropout layer of 0.5 rate and the ReLU activation function is applied. The aggregator type of each GraphSAGE layer is pooling, and the attention heads of GAT layer is set as 4. Note that the structure and hyperparameters used in this study proved to be sufficient for our applications, although they can still be improved.

### 4.4 Results

Table 3 shows the experiment results at AUC metrics. Reported numbers denote classification accuracy in percent. According to the experiment results, the OCGNN model achieve best results in all datasets. Among twelve the two-stage methods, only AE and PCA achieve competitive results in Pubmed dataset with raw features. The reason is that PCA and AE are better at processing high-dimensional original features. OCGNNs outperform than other two-stage methods, reaching the highest AUC improvement of above 30% than OCSVM in Cora and Citeseer dataset. Between three paradigms of OCGNNs, we believe that OC-GraphSAGE is the most powerful and stable one, because OC-GraphSAGE has great robustness thanks to its simple neighbor aggregation strategy.

We performed a T-SNE [Maaten and Hinton, 2008] visualization analyses on the embeddings learnt by the OCGNN framework in order to better understand the properties. We focus our analysis exclusively on the Cora dataset and use GraphSAGE algorithm as a bone of OCGNN. The reasons are that Cora dataset has the smallest number of nodes which can significantly aid clarity and GraphSAGE is a outstanding graph learning layer that is simple in form and has fewer hyperparameters. The embedding visualization in Fig. 1(a) and 1(b) indicates that we can not detect anomalous nodes by the raw node features or the initialized OCGNN. After 500 epochs of training, the normal and anomalous nodes seem to have a tendency to begin to separate. The KDE curves in Fig. 1(d) prove that where the probability density of normal nodes is high, the density of anomalous nodes is low, and vice versa. It means that a majority of normal and anomalous

| Method                      | Cora    | Citeseer | Pubmed   |
|-----------------------------|---------|----------|----------|
| DeepWalk                    | 57.87 ± 0.02 | 51.00 ± 0.03 | 60.73 ± 0.01 |
| DeepWalk + Raw Features     | 53.09 ± 0.03 | 46.33 ± 0.03 | 65.57 ± 0.02 |
| End-to-End (Our OCGNNs)     | 73.25 ± 0.02 | 62.81 ± 0.01 | 54.53 ± 0.01 |

Table 3: Average AUCs in % with StdDevs (over 10 random seeds). Note that the best result is typeset in **bold**.
Figure 1: T-SNE visualization of the node embeddings in Cora dataset. The KDE curves at top and right show the probability distribution in each dimension. Blue and orange points represent the normal nodes and the anomalous nodes, respectively. (a) The visualization of nodes’ raw features. (b) The visualization of node embeddings from a randomly initialized OCGNN model. (c) Node embeddings after 500 epochs training. (d) Node embeddings from a learned OCGNN model. We can conclude that OCGNN does learn the features of normal nodes and can distinguish abnormal nodes in an unsupervised manner.

Figure 2: The heatmap of average AUCs (%) of diverse OCGNN models in Cora dataset. The abscissa represents the dimensions of the hidden layer, and the ordinate represents the number of layers in the network. The lighter the color, the higher the performance of the model. Basically, the performance of the OCGNN model is robust to the structure of the network.

nodes can be easily partitioned in the embedding space, if the model converges.

4.5 Robustness

To verify the impact of network structure on performance, we tune the number of hidden layers from 1 to 7 and adjust the number of hidden neurons from 16 to 128, respectively. The results are shown in heatmap Figure 2. OCGNN’s performance will decrease when the size of the network is too large (top right) or too small (bottom left). The best results are usually obtained with a 2- to 4-layer model and 16 or 32 dimensions. When the network capacity is extremely small (1 hidden layer and 16 dimensions), the performance of OCGNN is greatly reduced because the insufficient networks cannot learn enough information of the normal training data. On the other hand, OCGNNs achieve slightly worse results when the network is too deep or too wide. A deep GNN model usually suffers from the over-smooth problem [Xu et al., 2018] because GNN models iteratively aggregate the node information of almost the entire graph layer by layer, and calculate node embeddings of low diversity. If the network is too wide, curse of dimensionality will cause OCGNN to fail in calculating distance terms in the loss function, because the distances of data points are approaching the same in high-dimensional space. As long as the scale of neural network is large enough, the number of network layers or the number of neurons will not have a significant impact on the results.

5 Conclusion

In this paper, we have proposed One Class Graph Neural Network (OCGNN), a one-class classification framework for graph anomaly detection. OCGNN aims at mapping the training nodes into a hypersphere in the embedding space, through the powerful representation ability of Graph Neural Networks. The results demonstrate that the proposed OCGNN achieves significant improvements in extensive experiments. Given that OCGNN currently only solves the problem of node anomaly detection, we will generalize OCGNN into graph-level anomaly detection in the future.

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