AEGCN: An Autoencoder-Constrained Graph Convolutional Network

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Abstract

We propose a novel neural network architecture, called autoencoder-constrained graph convolutional network, to solve node classification task on graph domains. As suggested by its name, the core of this model is a convolutional network operating directly on graphs, whose hidden layers are constrained by an autoencoder. Comparing with vanilla graph convolutional networks, the autoencoder step is added to reduce the information loss brought by Laplacian smoothing. We consider applying our model on both homogeneous graphs and heterogeneous graphs. For homogeneous graphs, the autoencoder approximates the adjacency matrix of the input graph by taking hidden layer representations as encoder and another one-layer graph convolutional network as decoder. For heterogeneous graphs, since there are multiple adjacency matrices corresponding to different types of edges, the autoencoder approximates the feature matrix of the input graph instead, and changes the encoder to a particularly designed multi-channel pre-processing network with two layers. In both cases, the error occurred in the autoencoder approximation goes to the penalty term in the loss function. In extensive experiments on citation networks and other heterogeneous graphs, we demonstrate that adding autoencoder constraints significantly improves the performance of graph convolutional networks. We also notice that such technique can be applied on graph attention network to improve the performance as well. This reveals the wide applicability of the proposed autoencoder technique.

Keywords: Homogeneous and heterogeneous graphs; Graph convolutional networks; Graph autoencoder; Graph node classification

1 Introduction

The complex relationships among data can be represented by networks in a variety of scientific areas, ranging from molecular biology (Mitchell et al., 1990; Jacobs et al., 2001; Higham et al., 2008), molecular chemistry (Balasubramanian, 1985; Balaban, 1985), genetics (Nordborg, 2000; Garway et al., 2008) to sociology (Ugander et al., 2011; Scott, 2012). Correspondingly, we have protein networks, atom networks, gene networks, and social networks. All these networks data can be structured as graphs. However, in many applications, graphs tend to be high-dimensional and highly entangled. Therefore, how to extract the structural information efficiently is always of central interest.

One of the most notable ways is graph representation learning, which aims to map nodes’ high-dimensional representations to low-dimensional vectors and, meanwhile, to preserve the structural
information as much as possible. The learned low-dimensional vectors, also called embedding vectors (or embeddings), are capable to benefit a wide range of downstream machine learning tasks, such as link prediction (Taskar et al., 2004; Al Hasan and Zaki, 2011; Gao et al., 2011), node classification (Bhagat et al., 2011; Tang et al., 2016), clustering (Tian et al., 2014), community detection (Fortunato, 2010), and visualization (van der Maaten and Hinton, 2008).

Existing methods of graph representation learning may be categorized into three types:

(a) \textit{random walk-based algorithms}: DeepWalk (Perozzi et al., 2014) is regarded as the first widespread embedding method. It interprets the co-occurrence nodes in a random walk as the “context”, applies SkipGram model (Mikolov et al., 2013) on the generated random walks, and maximizes the log-likelihood of observed context nodes. Node2vec (Grover and Leskovec, 2016) further extends the idea by proposing a biased random walk algorithm with two hyper-parameters, which balances the exploration-exploitation trade-off and integrates the homophily and structural equivalence of the network into the embeddings. LINE (Tang et al., 2015b) upgrades DeepWalk by defining a novel loss function to preserve both first- and second-order proximity between nodes, and subsequently its extension, PTE (Tang et al., 2015a), is developed targeting heterogeneous graphs. See Dong et al. (2017); Fu et al. (2017); Wang et al. (2017a) for more related algorithms and Cai et al. (2018) for a brief survey.

(b) \textit{matrix factorization-based algorithms}: graph embedding has also been investigated through the lens of matrix factorization. For example, Tang and Liu (2009, 2011) factorize the modularity matrix, which is an effective community measure for many complex networks (Newman, 2006). Cai et al. (2011); Dong et al. (2016) factorize the (normalized) Laplacian matrix. Yang et al. (2017); Ou et al. (2016) factorize different types of similarity matrices. Moreover, Qiu et al. (2018); Liu et al. (2019) provide some theoretical connections between random walk-based algorithms and the spectral theory of graph Laplacian. It is known that DeepWalk is equivalent to implicit matrix factorization on the normalized Laplacian matrix.

(c) \textit{graph neural networks (GNNs)}: GNNs are deep learning-based methods that operate directly on graph domains, which have become popular graph analysis methods due to the magnificent performance and the high interpretability. GNNs resolve two limitations of the above two categories: (i) no parameters are shared between nodes so that the problem scale grows linearly with respect to the number of nodes. (ii) the above two categorizes have limited generalization ability so that the learned embeddings perform poorly on new graphs. Motivated by the great success of standard NNs, researchers attempt to generalize NNs to corresponding GNNs. For concreteness, convolutional neural network (CNN) (Krizhevsky et al., 2012), recurrent neural network (RNN) (Schuster and Paliwal, 1997), and attention network (AN) (Vaswani et al., 2017) are generalized to graph convolutional network (GCN) (Kipf and Welling, 2016a), graph recurrent neural network (GRNN) (Li et al., 2015; You et al., 2018), and graph attention network (GAN) (Veličković et al., 2017), respectively. In addition, graph convolutional recurrent network (GCRN) (Seo et al., 2018) has also been developed and demonstrated ground-breaking performance on graph data. We point the reader to Zhou et al. (2018) for a recent overview of GNNs. Our paper is closely related to GCN, and more detailed related literature on GNN will be discussed later.

In this manuscript, we complement the third category by a novel GNN architecture, called autoencoder-constrained graph convolutional network (AEGCN). As suggested by its name, our model has two components:

(a) \textit{GCN}: the fundamental thread of our model is GCN, which takes feature matrix and adjacency
(b) **graph autoencoder**: within GCN, we add a graph autoencoder layer to impose some implicit constraints on hidden layers. In particular, the encoder is hidden layer representations while the decoder is one-layer GCN. The autoencoder in our model is used to approximate either adjacency matrix (for homogeneous case) or feature matrix (for heterogeneous case) of the input graph. It guarantees that the hidden layer does not lose too much *node-level* information from the input, and is equivalent to constraining the hidden layer in a way that the *uniqueness* of each node is encoded properly. The autoencoder approximation error together with the GCN classification error forms the classification objective.

We implement the above model on both homogeneous graphs and heterogeneous graphs for solving node classification task. Comparing with vanilla GCN on homogeneous graphs, we show in experiments that adding an extra autoencoder layer significantly improves the performance. Moreover, we consider heterogeneous graphs that contain different types of nodes and edges. To this end, we design a multi-channel pre-processing network with two layers to compress multiple adjacency matrices to a single adjacency matrix, and apply autoencoder to approximate the feature matrix of the input graph. The experimental results back up the argument again that the hidden layer constraints can benefit the performance of GCN. Furthermore, we observe in implementations that our autoencoder technique can be effectively utilized on GAN as well, which reveals the wide applicability of our method.

**Motivation and contribution:** Our model architecture is motivated by recent understanding of GCN. GCN was first proposed in Kipf and Welling (2016a) for solving semi-supervised node classification problem for graph-structured data. It has then been applied on various application fields due to its simplicity and efficacy (Derr et al., 2018; Gao et al., 2018; Ying et al., 2018). In principle, GCN generalizes the convolution from Euclidean domain to graph domain. It applies Fourier transformation for both signal (or feature) and filter, multiplies them, and transforms the product back to the discrete domain. The transformation relies on the spectral decomposition of graph Laplacian. The low-rank approximation of decomposition is achieved using truncated Chebyshev polynomials. It is known that the benefits of GCN architecture arise from “local averaging” (or called Laplacian smoothing), brought by the linear approximation of graph convolution. However, there is a trade-off between graph-level information and node-level information.

In specific, Laplacian smoothing nicely integrates the local connectivity patterns by averaging the feature of each node with its neighbors’. The nodes in the same class tend to have a common feature after multi-layer convolutions, and the graph-level information is hence captured. However, a potential concern of such mechanism is *over-smoothing*. The smoothed features of nodes cannot reflect their uniqueness in the input graph, so that the node-level information is not thoroughly encoded within GCN, which in turn limits the performance of GCN. Motivated by such limitation, we complement GCN with an additional autoencoder layer. The goal of this layer is to reduce the deviation between the hidden layer representations and the original representations, so that the network can preserve much node-level information.

Autoencoder, consisting of encoder and decoder, is a widely used dimension reduction framework. In encoder step, it maps high-dimensional representations to low-dimensional embeddings, while in decoder step, it solves downstream tasks by particular models with embeddings from the encoder step, defines the proper loss function, and trains parameters in both steps. In the present paper, the downstream task is to preserve the node-level information, which is characterized by the
approximation to either adjacency matrix or feature matrix. The encoder is naturally given by the hidden layer of GCN, while the decoder we choose is another layer of GCN. We interpret the approximation error as the regularization term in the loss function. Intuitively, in our model, GCN learns the graph-level information by Laplacian smoothing, while autoencoder provides some implicit constraints to alleviate the loss of node-level information.

The main contributions of the paper are three-fold. First, we propose a novel GCN-based network architecture, AEGCN, and apply it on homogeneous graphs. To the best our knowledge, AEGCN is the first algorithm that restricts the hidden layer in a way to avoid over-smoothing, by the aid of the autoencoder framework. The experimental results on citation networks show that AEGCN outperforms other state-of-the-art GCN-based methods. Second, we adjust GCN and the autoencoder technique to fit in the heterogeneous case. We design a multi-channel GCN and, relying on the weighted matrix product of different types of adjacency matrices, obtain a single adjacency matrix, each element of which corresponds to a length-2 meta-path between two nodes. We show in experiments that our model achieves the best performance on multiple heterogeneous graph datasets. Third, we apply the same idea on graph attention network. We observe that the constrained graph attention network also outperforms the original one. This demonstrates the considerable potential of our technique.

Relationship to literature: Our work is related to three active research lines. First, we contribute to the growing literature on GNNs. Like other deep learning models, GNNs achieve very promising results on different tasks and have strong generalization ability. Recent developments on optimization techniques and parallel computation have enabled efficient training on them. As one of the first widespread GNN models, a large body of literature have studied GCN and developed different extensions. For example, Li et al. (2018b) designs an adaptive GCN model, which is able to take graphs with arbitrary size and connectivity pattern as inputs. Abu-El-Haija et al. (2018) aggregates GCN by the information contained in random walks, and generates and trains multiple GCN instances over node pairs for node classification. Zhao et al. (2019) proposes a temporal GCN model by combining GCN with gated recurrent unit, and applies the model on intelligent traffic systems. In order to improve training efficiency, Chen et al. (2018) interprets the graph convolution as the integral of the embedding function under certain probability measure, and uses the importance sampling to estimate the integral. Wu et al. (2019) reduces the complexity of GCN by removing nonlinearities in hidden layers, and illustrates on multiple datasets that such reduction does not negatively affect the accuracy. He et al. (2020) also reports LightGCN model to simplify GCN, which only includes the neighborhood aggregation part. Our paper complements the aforementioned GCN-based models with AEGCN, which is the first GCN architecture regularized by autoencoder. Instead of simplifying GCN, we aim to address the over-smoothing issue of GCN via the autoencoder technique.

Second, our work is related to graph autoencoder. Recently, there has been much interest on studying the framework of autoencoder for graph embedding. Kipf and Welling (2016b) designs an unsupervised autoencoder framework for graphs with a GCN encoder and an inner product decoder. Berg et al. (2017) designs an autoencoder to handle link prediction of the bipartite interaction graphs, and applies it on solving matrix completion problems. Wang et al. (2017b) proposes a marginal graph self-encoder algorithm for graph clustering problem. Pan et al. (2018) encodes the topology and node content of the graph into a compact representation, and proposes adversarial graph autoencoder framework via the adversarial training scheme. Na et al. (2020) formalizes the embedding problem as a statistical estimation problem, proposes a semiparametric decoder model,
and uses a pseudo-likelihood objective to solve the embedding problem for bipartite graphs. We refer to Hamilton et al. (2017) for a survey on graph autoencoder. Comparing with the above work, our paper heuristically exploits autoencoder on constraining the hidden layers of GCN. The goal of autoencoder in our model is not node classification, which is addressed by GCN, but the approximation to node-level information of the input graph. This implementation of autoencoder has not been considered in the previous work.

Third, our work is related to the literature on understanding the mechanism of GCN. Li et al. (2018a) argues that GCN model is actually a special form of Laplacian smoothing, which is the key reason why GCN works, while in turn results in a concern of over-smoothing. Kampffmeyer et al. (2019) studies the trade-off between breadth and depth of GCNs, and adds multiple edges on the original tree-structured data to make it dense to balance the trade-off. However, their method significantly enhances the training difficulty due to the increase of the problem scale. We contribute this series of work by proposing a cheap solution to the potential over-smoothing issue. We argue that combining autoencoder regularization with GCN is able to effectively avoid over-smoothing of GCN, and such technique is also worth trying for other network architectures.

Throughout the presentation, we let $|V|$ be the cardinality of the set $V$. By $I_n$ we denote the $n \times n$ identity matrix. For a sequence of matrices $A_i \in \mathbb{R}^{n \times d_i}$, $|I| A_i \in \mathbb{R}^{n \times \sum d_i}$ denotes the matrix obtained by concatenating $A_i$ by column sequentially.

Structure of the paper: In Section 2, we introduce some preliminaries including homogeneous and heterogeneous graphs, GCN and autoencoder. In Section 3, we introduce our model. The experimental results are demonstrated in Section 4 and conclusions and future work are summarized in Section 5.

2 Preliminaries

Before introducing our method, we begin with some preliminaries. We first introduce homogeneous graphs and heterogeneous graphs, then present how GCNs implement on homogeneous graphs, and then introduce the autoencoder framework.

Let $G = (V, E)$ be a graph where $V = \{v_1, \ldots, v_n\}$ is a set of nodes and $E$ is a set of edges. We say it is a homogeneous graph if it has a single type of node and a single type of edge, otherwise it is a heterogeneous graph. The former definition is as follows.

Definition 2.1. Given a graph $G = (V, E)$, we let $f^V : V \rightarrow \mathcal{T}^V$ be a node type mapping function and $f^E : E \rightarrow \mathcal{T}^E$ be an edge type mapping function, where $\mathcal{T}^V$ and $\mathcal{T}^E$ are the predefined nonempty node types set and edge types set. $G$ is called a homogeneous graph if $|\mathcal{T}^V| + |\mathcal{T}^E| = 2$, a heterogeneous graph if $|\mathcal{T}^V| + |\mathcal{T}^E| > 2$.

In the above definition, we implicitly assume there exists at least one edge on the graph. In general, heterogeneous graphs (Sun et al., 2011, 2013) contain more comprehensive structured relations (edges) among nodes and unstructured contents (features) associated with each node. For example, features of different types of nodes may fall in different spaces, and two nodes may be connected via different semantic paths, called meta-paths. We demonstrate the differences of two types of graphs by the example in Figure 1.

In Figure 1(a), we construct a homogeneous graph to model Cora citation network (Sen et al., 2008). It contains a single node type (paper) and a single edge type (reference relationship). In Figure 1(b), we construct a heterogeneous graph to model ACM citation network. It contains
three node types: author, paper, and subject, and four edge types: author-paper, paper-author, paper-subject and subject-paper. For this graph, we see that there are two meta-paths between two paper nodes: paper-author-paper and paper-subject-paper. The former indicates two papers have the same author, while the latter indicates two papers belong to the same subject. Such information can not be represented in a homogeneous graph.

For clarity, we further introduce the notations of adjacency matrix and degree matrix.

**Definition 2.2.** Given a graph $G = (V, E)$ with $|V| = n$ and $|E|$ being the edge types set, we let $A = \{A_k\}_{k=1}^{|E|}$ be the adjacency matrices class, where $A_k \in \mathbb{R}^{n \times n}$ with $(A_k)_{ij} = 1$ if there exists a type $k$ edge between node $i$ and node $j$, otherwise $(A_k)_{ij} = 0$. When $|E| = 1$, $A$ has a single adjacency matrix, denoted by $A$. Moreover, for an adjacency matrix $A$, $\tilde{A} = A + I_n$ is the adjacency matrix with self-connections, and the diagonal matrix $\tilde{D} \in \mathbb{R}^{n \times n}$, with $\tilde{D}_{ii} = \sum_{j=1}^{n} \tilde{A}_{ij}$, is the degree matrix of $\tilde{A}$.

We now set the stage for introducing the graph convolutional network (GCN) on homogeneous graphs. Suppose $A \in \mathbb{R}^{n \times n}$ and $X \in \mathbb{R}^{n \times d}$ are the adjacency matrix and the feature matrix of the graph $G$, respectively, GCN has the following propagation rule:

$$
\begin{align*}
H^{(l+1)} &= \sigma \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right), \quad l = 0, 1, \ldots, \\
H^{(0)} &= X,
\end{align*}
$$

(1)

where $\sigma(\cdot)$ is some nonlinear activation functions, $H^{(l)} \in \mathbb{R}^{n \times d_l}$ is the input activation matrix of the $l$-th hidden layer, $W^{(l)} \in \mathbb{R}^{d_l \times d_{l+1}}$ is the trainable weight matrix with $d_0 = d$. Here, each row of $H^{(l)}$ corresponds to the representation of each node in the hidden layer. The matrix $\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}}$ comes from applying normalization trick on the convolution matrix $I_n + D^{-\frac{1}{2}} \tilde{A} D^{-\frac{1}{2}}$, where $D$ with $D_{ii} = \sum_{j=1}^{n} \tilde{A}_{ij}$ is the degree matrix of $A$. The motivation of the rule in (1) is referred to Kipf and Welling (2016a); Li et al. (2018a). One can show that the convolution on $H^{(l)}$, $\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)}$, is equivalent to performing the Laplacian smoothing on each channel of $H^{(l)}$ (Taubin, 1995), so that the deviation among representations of $H^{(l)}$ will be moderated in $H^{(l+1)}$.

For notation simplicity, we use $\text{GCN}(X, A)$ to denote the output of a GCN model with inputs $X$ and $A$. The number of layers and the choice of activation functions are suppressed in the notation.
The standard (non-probabilistic) graph autoencoder model (Kipf and Welling, 2016b) consists of a GCN encoder model and a nonlinear inner product decoder model. The task of decoder is to reconstruct adjacency matrix $A$. In particular, the autoencoder can be summarized as

Encoder: $Z = \text{GCN}(X, A)$,

Decoder: $\hat{A} = \sigma(ZZ^T)$. \hfill (2)

Our method will replace the decoder model by another layer of GCN.

3 Autoencoder-constrained GCN

This section presents our model. We handle the homogeneous graph first to warm up. The core of our model is GCN, which is used to perform node classification task. We use a two-layer GCN architecture to illustrate the main idea.

Given a homogeneous graph $G = (V, E)$, we suppose $A \in \mathbb{R}^{n \times n}$ is its adjacency matrix, $X \in \mathbb{R}^{n \times d}$ is its feature matrix, and $Y \in \mathbb{R}^{n \times f}$, defined as $Y_{ij} = 1$ if node $i$ belongs to class $j$ and $Y_{ij} = 0$ otherwise, is the label matrix. Following the rule in (1), two-layer GCN takes the form

$H^{(1)} = \text{ReLU} \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} X W^{(0)} \right)$,

$H^{(2)} = \text{softmax} \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(1)} W^{(1)} \right)$.

Here, $W^{(0)} \in \mathbb{R}^{d \times d_1}$ and $W^{(1)} \in \mathbb{R}^{d_1 \times f}$ are weight matrices for two layers, $\text{ReLU}(\cdot) = \max(0, \cdot)$ is applied entry-wise, the softmax activation function, defined as $(\text{softmax}(Z))_i = \frac{1}{Z} \exp(Z_i)$ with $Z = \sum_i \exp(Z_i)$, is applied row-wise. Based on the output $H^{(2)}$, the classification error is defined by the cross-entropy loss:

$L_{\text{class}} = -\frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{f} Y_{ij} \log H_{ij}^{(2)}$. \hfill (3)

On the other hand, since hidden layer representation $H^{(1)}$ is obtained by doing Laplacian smoothing on $X$, the node-level information of $X$ is depressed in this step. We adopt the autoencoder framework to compensate for such information loss. The encoder model is simply given by $H^{(1)}$, while different from (2), the decoder model is another layer of GCN. We have

$\hat{A} = \text{sigmoid} \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(1)} W^{(a)} \right)$.

Here $W^{(a)} \in \mathbb{R}^{d_1 \times n}$ and sigmoid function is applied entry-wise. We adopt sigmoid instead of softmax as activation function since comparing the output of the decoder with the (normalized) adjacency matrix can be viewed as a multi-label classification task. We realize in implementation that the above decoder model performs better than (2) on both GCN and GAN architectures. We then measure the autoencoder approximation error by cross-entropy loss again:

$L_{\text{auto}} = -\frac{1}{n^2} \sum_{i,j=1}^{n} (\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}})_{ij} \log \hat{A}_{ij}$. \hfill (4)
Combining two loss functions in (3) and (4), we train $W^{(0)}, W^{(1)}, W^{(a)}$ by performing gradient descent on the penalized loss function

$$\mathcal{L} = \mathcal{L}_{\text{class}} + \gamma \mathcal{L}_{\text{auto}}$$

with tuning parameter $\gamma$. The above network architecture is illustrated in Figure 2.

![Figure 2: Illustration of AEGCN on homogeneous graphs. The top thread is two-layer GCN, while the bottom thread is autoencoder.](image)

Following the same flavor, we consider the heterogeneous graphs. For a heterogeneous graph $G = (V, E)$, we let $X \in \mathbb{R}^{n \times d}$ and $Y \in \mathbb{R}^{n \times f}$ be the feature matrix and label matrix, respectively, and $A = \{A_k\}_{k=1}^{\lvert T_E \rvert}$ be the adjacency matrices class. The idea is to transform $A$ to a single adjacency matrix and apply the same model for the homogeneous case. Inspired by Yun et al. (2019), we transform $A$ by two graph transformer layers.

In the first layer, we first generate multiple new graphs defined by the convex combination of adjacency matrices in $A$. Then, we aggregate graphs to a single graph and use its adjacency matrix as our single adjacency matrix. We make use of the weighted matrix product, so that each entry of the single adjacency matrix corresponds to a meta-path. In particular, we generate $C$ pairs of graph structures from $A$ by

$$Q_1^i = \sum_{k=1}^{\lvert T_E \rvert} (\tilde{W}_1^i)_k \cdot A_k \quad \text{and} \quad Q_2^i = \sum_{k=1}^{\lvert T_E \rvert} (\tilde{W}_2^i)_k \cdot A_k, \quad \text{for } i = 1, \ldots, C,$$

where $\tilde{W}_j^i = \text{softmax} \left( W_j^i \right) \in \mathbb{R}^{\lvert T_E \rvert}$ for $j = 1, 2$ are coefficients of the convex combination. Here, $\{W_1^i, W_2^i\}_{i=1}^C$ are weights to be optimized. Given a pair $(Q_1^i, Q_2^i)$, $A^i = Q_1^i Q_2^i$ represents the adjacency matrix of length-2 meta-paths. We further let $A^i = A^i + I_n$ and the single adjacency matrix is defined as

$$\tilde{A}_H = \sum_{i=1}^C A^i.$$
In the second layer, we aggregate the features by one convolutional layer:

\[ H^{(0)} = \left| \bigcup_{i=1}^{C} ReLU \left( \tilde{D}_i^{-1} \tilde{A}_i X W^{\text{aggre}} \right) \right], \]

where \( \tilde{D}_i \) is the degree matrix of \( \tilde{A}_i \) and \( W^{\text{aggre}} \) is a trainable weight matrix shared across channels.

Using \( \tilde{A}_H \) and \( H^{(0)} \) and letting \( \tilde{D}_H \) be the degree matrix of \( \tilde{A}_H \), we follow the previous AEGCN architecture:

\[
\text{GCN} : \quad H^{(1)} = ReLU \left( \tilde{D}_H^{-1} \tilde{A}_H H^{(0)} W^{(0)} \right), \\
H^{(2)} = \text{softmax} \left( H^{(1)} W^{(1)} + b \right), \\
\text{Autoencoder} : \quad \hat{X} = \text{sigmoid} \left( \tilde{D}_H^{-1} \tilde{A}_H H^{(0)} W^{(a)} \right).
\]

Moreover, the classification error is same as (3), while the autoencoder approximation error is redefined as

\[
\mathcal{L}_{\text{auto}} = -\frac{1}{nd} \sum_{i=1}^{n} \sum_{j=1}^{d} X_{ij} \log \hat{X}_{ij}.
\]

Combining loss functions \( \mathcal{L}_{\text{class}} \) and \( \mathcal{L}_{\text{auto}} \), we perform gradient descent to optimize all weight matrices \( \{W_i, W_2\}^{C}_{i=1}, W^{\text{aggre}}, W^{(0)}, W^{(1)}, W^{(a)} \). We illustrate the heterogeneous case in Figure 3.

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**Figure 3:** Illustration of AEGCN on heterogeneous graphs. The top thread is two-layer GCN, while the bottom thread is autoencoder. The right part from \( H^{(0)} \) is consistent with Figure 2, while the left part is two graph transformer layers.

**Remark 3.1.** There are two main differences between models in heterogeneous case and in homogeneous case. In heterogeneous case, our autoencoder approximates the original feature matrix \( X \) instead of the adjacency matrix. The reason is that \( \tilde{A} \) contains different types of adjacency matrices, and it’s not clear to us which single adjacency matrix, including \( \tilde{A}_H \), can reflect the most node-level information of the input graph. Further, in graph convolution, we use the asymmetric in-degree matrix \( \tilde{D}_H^{-1} \) to normalize the adjacency matrix, rather than \( \tilde{D}_H^{-1/2} \) in homogeneous case. This is because most of heterogeneous graphs (e.g. ACM networks and IMDB networks) are directed and symmetric normalization is not suitable.
4 Experiments

In this section, we conduct extensive experiments on real benchmarks to testify the proposed method. We also extend our autoencoder regularization idea to graph attention network (GAN) and study the applicability of such technique on different network architectures. Our code is publicly available at https://github.com/AI-luyuan/aegcn.

4.1 Homogeneous graphs

We conduct experiments on three commonly used citation networks: Cora, Citeseer, and Pubmed (Sen et al., 2008). These networks contain only one node type (paper) and one edge type (reference relationship), thus they are homogeneous graphs. The statistics are summarized in Table 1.

| Dataset | #Nodes | #Edges | #Classes | #Features | #Training | #Validation | #Test |
|---------|--------|--------|----------|-----------|-----------|-------------|-------|
| Cora    | 2708   | 5429   | 7        | 1433      | 140       | 500         | 1000  |
| Citeseer| 3327   | 4732   | 6        | 3703      | 120       | 500         | 1000  |
| Pubmed  | 19717  | 44338  | 3        | 500       | 60        | 500         | 1000  |

We compare our method with several state-of-the-art baselines listed in Table 2, including some GCN-based methods, GAN, DeepWalk, and a semi-supervised embedding method.

- SemiEmb: A nonlinear semi-supervised embedding algorithm that applies “shallow” learning techniques such as kernel methods on deep network architectures, via adding a regularizer at the output layer.
- DeepWalk: A random walk-based embedding algorithm that applies SkipGram model on the generated random walks and maximizes the log-likelihood objective.
- GAN: A semi-supervised GNN that generalizes the attention network on graph-structured data.
- GCN: A semi-supervised GNN that generalizes the convolutional network on graph-structured data.
- FastGCN: A GCN-based method that treats the graph convolution as an integral of embedding functions under certain probability measures, and applies importance sampling to estimate the integral.
- SGCN: A simplified GCN architecture by successively removing nonlinearities and collapsing weight matrices between consecutive layers.
- RGCN: A robust GCN method that is able to absorb the effects of adversarial attacks on the graph by assuming nodes representations of hidden layers follow Gaussian distribution.

**Implementation details:** As described in Section 3, our model consists of two GCN layers and one autoencoder layer. We use the same data splitting as in Yang et al. (2016) as shown in Table 1. For all datasets, we train the model for 200 epochs, tune hyperparameters, including hidden layer dimension, learning rate, dropout rate and weight decay, for Cora dataset only, and use the same set of parameters for Citeseer and Pubmed. The hidden layer dimension $d_1$ is set to be 18 and, same as Kipf and Welling (2016a), the learning rate, dropout rate, weight decay are set to be
Table 2: Descriptions of baseline models for homogeneous graphs

| Model                  | Short description                              |
|------------------------|------------------------------------------------|
| SemiEmb (Weston et al., 2012) | Deep learning via semi-supervised embedding |
| DeepWalk (Perozzi et al., 2014) | Random walk-based network embedding method   |
| GAN (Veličković et al., 2017) | Graph attention network                       |
| GCN (Kipf and Welling, 2016a) | Graph convolutional network                    |
| FastGCN (Chen et al., 2018) | Fast learning with GCN via importance sampling |
| SGCN (Wu et al., 2019) | Simplifying graph convolutional network       |
| RGCN (Zhu et al., 2019) | Robust graph convolutional network             |

0.01, 0.5, 0.0005, respectively. We set $\gamma = 10$ for Core and Citeseer, and set $\gamma = 0.001$ for Pubmed. All results are reported over 30 independent runs. The results for all other baselines are directly borrowed from Kipf and Welling (2016a); Wu et al. (2019); Zhu et al. (2019).

**Experimental results:** The results are summarized in Table 3. From the table, we find that GNN methods enjoy significantly better performance than SemiEmb and DeepWalk. Comparing within GNNs, AEGCN has consistently better results on all three datasets than GCN, FastGCN, and SGCN. RGCN performs slightly better than AEGCN on Cora network, while in turn AEGCN outperforms it on the other two networks. By simple calculations, we see that our simple autoencoder constraint framework can improve the accuracy of other GCN-based methods by 0.2% to 3.5%. This suggests the effectiveness of the introduced autoencoder constraints. As for efficacy, we find that AEGCN only adds one GCN layer compared to the vanilla GCN, so they have comparable running time. It is worth mentioning that GAN has better results on Cora and Citeseer networks, however the running time is significantly longer than all other GCN-based methods.

Table 3: Comparison results of homogeneous graphs

| Method  | Cora     | Citeseer | Pubmed   |
|---------|----------|----------|----------|
| SemiEmb | 59.0     | 59.6     | 71.1     |
| DeepWalk | 67.2     | 43.2     | 65.3     |
| GCN     | 81.5     | 70.3     | 79.0     |
| GAN     | 83.0 ± 0.7 | 72.5 ± 0.7 | 79.0 ± 0.3 |
| FastGCN | 79.8 ± 0.3 | 68.8 ± 0.6 | 77.4 ± 0.3 |
| SGCN    | 81.0 ± 0.0 | 71.9 ± 0.1 | 78.9 ± 0.0 |
| RGCN    | 82.8 ± 0.6 | 71.2 ± 0.5 | 79.1 ± 0.3 |
| AEGCN   | 82.4 ± 0.7 | 72.3 ± 0.6 | 79.3 ± 0.1 |

### 4.2 Heterogeneous graphs

We consider two heterogeneous graphs: ACM citation network and IMDB movie network. ACM contains three types of nodes (paper, author, subject), and four types of edges (paper-author, author-paper, paper-subject, subject-paper). The category of the paper is the label, and the feature of each node is given by bag-of-words of keywords. IMDB contains three types of nodes (movie, actor, director), and four types of edges (movie-actor, actor-movie, movie-director, director-movie). The
genre of the movie is the label, and the feature of each node is given by bag-of-words representations of plots. The statistics of two datasets are summarized in Table 4.

Table 4: Statistics of heterogeneous graphs

| Dataset | #Nodes | #Edges | #Edge type | #Features | #Training | #Validation | #Test |
|---------|--------|--------|------------|-----------|-----------|-------------|-------|
| ACM     | 8994   | 25922  | 4          | 1902      | 600       | 300         | 2125  |
| IMDB    | 12772  | 37288  | 4          | 1256      | 300       | 300         | 2339  |

In this part, we compare with four baselines listed in Table 5. The GCN-based baselines in Table 2 are not implemented here since they are particularly designed for homogeneous graphs, and it’s not clear how to fairly adapt them to heterogeneous graphs.

• metapath2vec: A random walk-based embedding method for heterogeneous networks, which constructs the heterogeneous neighborhood of a node by performing meta-path-based random walks, and hinges on a heterogeneous SkipGram model to compute embeddings.

• HAN: A semi-supervised GNN for heterogeneous network which generates node embedding by aggregating features from meta-path-based neighbors in a hierarchical manner to employ both node-level attention and graph-level attention.

• GTN: A supervised GNN for heterogeneous network which generates multiple meta-paths by matrix multiplication, applies GCN on each path, and stacks all learned embeddings.

Table 5: Descriptions of baseline models for heterogeneous graphs

| Model               | Short description                           |
|---------------------|--------------------------------------------|
| DeepWalk (Perozzi et al., 2014) | Random walk-based network embedding method |
| metapath2vec (Dong et al., 2017)  | Random walk-based network embedding method |
| HAN (Wang et al., 2019)       | GNN for heterogeneous graph                |
| GTN (Yun et al., 2019)        | GNN for heterogeneous graph                |

Implementation details: As described in Section 3, our model consists of two pre-processing graph transformer layers, two GCN layers, and one autoencoder layer. We use the same data splitting as in Yun et al. (2019) as shown in Table 4. We train the model with a maximum of 40 epochs, tune hyperparameters for ACM dataset, and use the same set of parameters for IMDB. The hidden layer dimensions \(d_0\) (columns of \(H^{(0)}\)) and \(d_1\) (columns of \(H^{(1)}\)), and the number of channels \(C\) are set to be 128, 64 and 2. The learning rate and weight decay are set to be 0.005, 0.001, respectively. Same as GTN, dropout technology is not used for AEGCN in the experiment. We set \(\gamma = 1\) for both ACM and IMDB. Results are reported over 10 independent runs. Results for DeepWalk, metapath2vec and HAN are borrowed from Yun et al. (2019). Results for GTN are reported using the source code from Yun et al. (2019) under the same parameters setup and same experimental environment.

Experimental results: The results are summarized in Table 6. From the table, we see AEGCN has the best performance on both datasets. DeepWalk and metapath2vec perform worse than GNN methods. Although HAN is a modified GAN for heterogeneous graph, the GCN-based models, GTN and AEGCN, perform better than HAN, which is different from the results of previous subsection.
By Table 6, we reach the same conclusion that the proposed architecture is effective for solving node classification task on heterogeneous graphs.

Table 6: Comparison with Baseline Models

| Dataset | DeepWalk | metapath2vec | HAN | GTN | AEGCN |
|---------|----------|--------------|-----|-----|-------|
| ACM     | 67.42    | 87.61        | 90.96| 92.68| 93.08 |
| IMDB    | 32.08    | 35.21        | 56.77| 57.29| 58.03 |

To have a closer view, we plot in Figure 4 the changes in Macro-F1 score during AEGCN and GTN training processes in two datasets. Macro-F1 score is a common metric to measure the accuracy of the classifier, which takes both precision and recall into account. In general, the higher the F1 score, the more accurate the classifier. However, one should be aware of an extremely high F1 score on the training set, which is generally due to the overfitting error. From two plots in Figure 4, we see that F1 score grows gradually during the training process of AEGCN, while it almost hits 1 after very few epochs for GTN. This observation suggests that our proposed regularized method can effectively postpone the occurrence of overfitting during the training. On the other hand, we also note that AEGCN has higher F1 score on the test set finally. Therefore, AEGCN is favored on both aspects.

![Figure 4: Macro-F1 score trajectories of GTN and AEGCN. The left panel is the result on ACM network, while the right panel is the result on IMDB network. For both panels, Tr_GTN and Tr_AEGCN correspond to the F1 score on the training set, while Te_GTN and Te_AEGCN correspond to the F1 score on the test set.](image)

4.3 Autoencoder on GAN

We apply our autoencoder regularization idea on GAN to explore the extensibility of our technique. We add the autoencoder layer on the hidden representations before the classification layer of GAN, and conduct experiments on citation networks. We let $\gamma = 1$ for all three networks and use the same parameters setting as Veličković et al. (2017). The results are reported over 10 runs.

The results are shown in Table 7. From the table, we see AEGAN performs better on Cora and Citeseer networks, while GAN performs better on Pubmed. Throughout the implementation, we simply use the original parameters of GAN with manually specified $\gamma$, and do not tune parameters.
Table 7: Comparison with GAN models

| Method  | Citeseer | Cora   | Pubmed  |
|---------|----------|--------|---------|
| GAN     | 72.5 ± 0.7 | 83.0 ± 0.7 | 79.0 ± 0.3 |
| AEGAN   | 72.6 ± 0.6 | 83.8 ± 0.3 | 78.5 ± 0.3 |

during the training. We believe that better results are achievable if we further tune parameters for AEGAN sophisticatedly.

This implementation shows that our autoencoder regularization framework not only benefits GCN, but also can migrate to other graph network architectures to improve the performance. This observation highlights the wide applicability and considerable potential of the proposed technique.

5 Conclusion and future work

In this paper, we propose a novel graph neural network architecture, called autoencoder-constrained graph convolutional network, abbreviated to AEGCN. The core of AEGCN is GCN, which is used to perform node classification task. Within GCN, we impose an autoencoder layer to reduce the loss of node-level information. The error occurred in the autoencoder step is treated as the regularizer of the classification objective. We apply our model on homogeneous graphs and heterogeneous graphs, and achieve superior performance on both cases over other competing baselines. We also apply our idea of autoencoder constraints on graph attention network, and find it can improve the performance of GAN as well. This observation reveals that our technique is applicable for a potentially wide range of network architectures.

Interesting future directions include studying the effectiveness of autoencoder constraints on other types of GNN architectures. In addition, the effects of the autoencoder regularization on deeper GNNs have to be further explored.

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