

Adaptive Graph Auto-Encoder for General Data Clustering

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Abstract

Graph based clustering plays an important role in clustering area. Recent studies about graph convolution neural networks have achieved impressive success on graph type data. However, in traditional clustering tasks, the graph structure of data does not exist such that the strategy to construct graph is crucial for performance. In addition, the existing graph auto-encoder based approaches perform poorly on weighted graph, which is widely used in graph based clustering. In this paper, we propose a graph auto-encoder with local structure preserving for general data clustering, which can update the constructed graph adaptively. The adaptive process is designed to utilize the non-Euclidean structure sufficiently. By combining generative model for graph embedding and graph based clustering, a graph auto-encoder with a novel decoder is developed and it performs well in weighted graph used scenarios. Extensive experiments prove the superiority of our model.

1. Introduction

Clustering, which intends to group data points without any prior information, is one of the most fundamental tasks in machine learning. As well as the well-known k-means, graph based clustering (Ng et al., 2002; Nie et al., 2014; Zhang et al., 2018) is also a representative kind of clustering method. A typical graph based clustering method includes two step: 1) construct graph by some algorithm; 2) divide samples into different clusters according to the constructed graph. For example, a classical spectral clustering method first builds a weighted adjacency matrix via k -nearest neighbors and Gaussian kernel, and then attempts to find a good graph cut to split the graph into multiple connected component. Accordingly, it is not hard to understand that the performance of these clustering methods depend severely on the quality of constructed graph. Graph based clustering methods are widely used since they can capture manifold information so that they are available for the non-Euclidean type data, which is not provided by k-means. Due to the success of deep learning, how to combine neural networks and traditional clustering model has been studied a lot (Sha-

ham et al., 2018; Xie et al., 2016; Zhang et al., 2019). In particular, the auto-encoder (Hinton & Salakhutdinov, 2006) is the base framework of most deep clustering approaches.

Network embedding (also known as graph embedding) is an attractive task for graph type data such as recommendation systems, social networks, *etc.* The goal is to map nodes of a given graph into latent features (namely embedding) so that the learned embedding can be utilized on node classification, node clustering and link prediction. Roughly speaking, the network embedding approaches can be classified into 2 categories: generative model (Wang et al., 2018; Perozzi et al., 2014; Grover & Leskovec, 2016) and discriminative model (Cao et al., 2016; Wang et al., 2016). The former tries to model a connectivity distribution for each node while the latter learns to distinguish whether edge exists between two nodes directly. Nevertheless, there is no method that aims at integrates generative models with clustering.

In recent years, graph neural networks (Scarselli et al., 2008), especially graph convolution neural networks (GCN), have attracted a mass of attentions due to the success made in neural networks area. GNNs extend classical neural networks to irregular data so that the deep information hidden in graph is exploited sufficiently. In this paper, we only focus on GCNs and its variants. Different from traditional CNNs, a key issue in GCN is how to define convolution operator on irregular data. An intuitive approach is to constrain neighbors of each node to perform convolution, which is frequently known as spatial method (Niepert et al., 2016). On the contrary, the spectral operator first defines frequency domain of graph data and then performs convolution with the help of convolution theorem. GCNs have shown superiority compared with traditional graph embedding models. Similarly, graph auto-encoder (Kipf & Welling, 2016) is developed to extend GCN into unsupervised learning.

However, the existing methods are limited to graph type data (*e.g.*, social networks, citation networks, *etc.*). Since a large proportion of clustering methods are based on graph like spectral clustering, it is reasonable to consider how to employ GCN to promote the performance of graph based clustering methods.

In this paper, we propose Adaptive Graph Auto-Encoder, a novel clustering model for general data clustering, to extend graph auto-encoder to common scenarios. The main

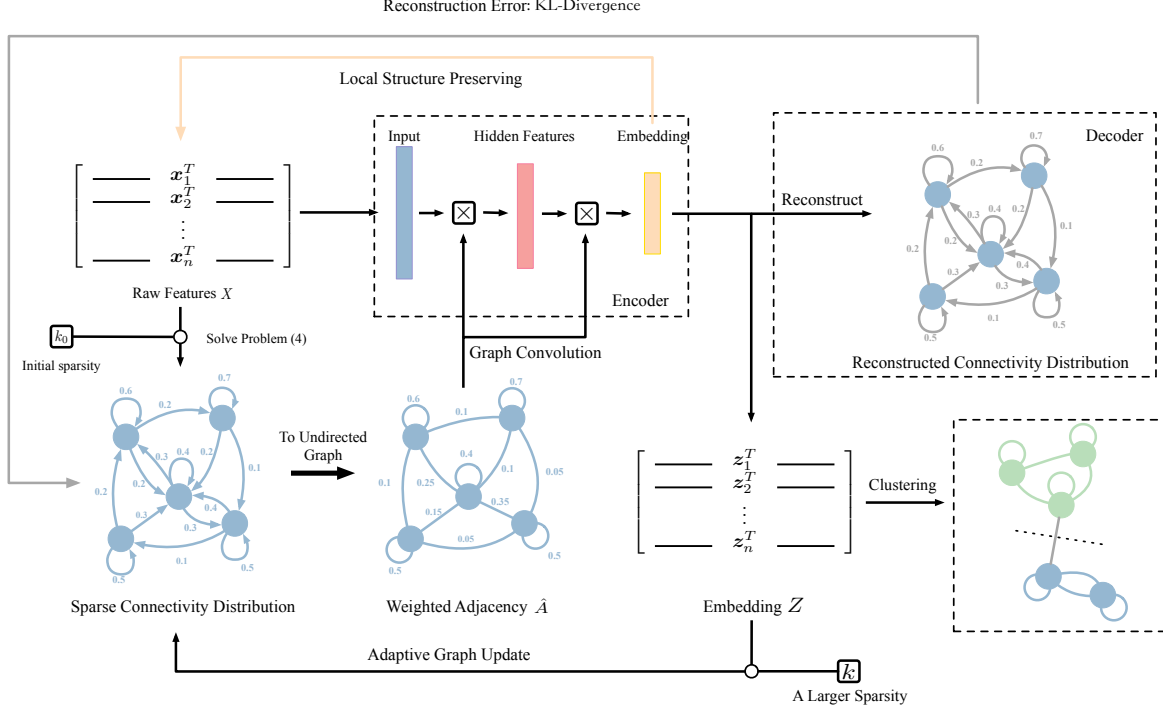


Figure 1. Illustration of AdaGAE

contributions are listed as follow

- To build a desirable graph, our model incorporates generative model of network embedding. Moreover, the learned connectivity distribution is also used as the goal that graph auto-encoder aims to reconstruct.
- Our model updates the graph adaptively according to the generated embedding so that it can exploit the deep information and revise the poor graph caused by raw features.
- Our models also employs a manifold regularization to preserve the local structure, which can be regarded as a pseudo-supervised information.

2. Preliminary and Related Work

We first introduce studies about graph convolution networks and graph auto-encoder. Generative graph representation models in network embedding are demonstrated roughly due to the connection between them and our model. Due to the limitation of space, classical clustering models (*e.g.*, spectral clustering) are omitted.

2.1. Notations

In this paper, matrices and vectors are represented by uppercase and lowercase letters respectively. For a square matrix

M , $tr(M)$ is the trace and M^T denotes the transpose of M . A graph is represented as $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{W})$ and $|\cdot|$ is the size of some set. Vectors whose all elements are 1 is represented as $\mathbf{1}$. If $\langle v_i, v_j \rangle \in \mathcal{E}$, then $\mathcal{W}_{ij} > 0$; otherwise, $\mathcal{W}_{ij} = 0$. For every node $v_i \in \mathcal{V}$, it is represented by a d -dimension vector x_i and thus, \mathcal{V} can be also denoted by $X = [x_1, x_2, \dots, x_n]^T \in \mathbb{R}^{n \times d}$. The amount of clusters is represented as c .

2.2. Graph Auto-Encoder

In recent years, graph convolution networks (*GCN*) have been studied a lot to extend neural networks to graph type data. How to design graph convolution operator is a key issue and has attracted a mass of attentions. Most of them can be classified into 2 categories, spectral methods (Niepert et al., 2016) and spatial methods (Bruna et al., 2013). In this paper, we focus on a simple but widely used convolution operator (Kipf & Welling, 2017), which can be regarded as both spectral operator and spatial operator. Formally, if the input of a graph convolution layer is $X \in \mathbb{R}^{n \times d}$ and the adjacency matrix is A , then the output is defined as

$$H = \varphi(\hat{A}XW) \quad (1)$$

where $\varphi(\cdot)$ is some activation function, $\hat{A} = \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}}$, $\tilde{A} = A + I$ and \tilde{D} denotes the degree matrix ($\tilde{D}_{ii} = \sum_{j=1}^n \tilde{A}_{ij}$). It should be pointed out that \tilde{A} can be regarded as a processed graph with self-loop for each node and \hat{A} is

the normalized adjacency matrix. More importantly, $\hat{A}X$ is equivalent to compute weighted means for each node with its first-order neighbors from the spatial aspect. To improve the performance, MixHop (Abu-El-Haija et al., 2019) aims to mix information from different order neighbors and SGC (Wu et al., 2019) tries to utilize higher-order neighbors. The capacity is also proved to some extent (Xu et al., 2019). GCN and its variants are usually used on semi-supervised learning. Besides, since training of each GCN layer needs all data to finish a complete propagation, several models are proposed to speed it up (Chen et al., 2018; Chiang et al., 2019).

To apply graph convolution on unsupervised learning, graph auto-encoder (GAE) is proposed (Kipf & Welling, 2016). GAE firstly transforms each node into latent representation (also named as embedding), which is similar with GCN, and then aims to reconstruct some part of input. GAEs proposed in (Kipf & Welling, 2016; Pan et al., 2018; Wang et al., 2019) intend to reconstruct the adjacency via decoder while GAEs developed in (Wang et al., 2017; Park et al., 2019) attempt to reconstruct the content. The difference is which extra mechanism (such as attention, adversarial learning, graph sharpness, etc.) is used.

2.3. Generative Graph Embedding

Graph representation learning is to transform nodes of graph into vector representation so that it can be employed to perform node classification, link prediction and so on. Similar with generative model in classical supervised learning, the core assumption of the generative model in network embedding is that there exists a underlying connectivity distribution and all edges in graph are sampled according to this true distribution. Therefore, the generative model intends to approximate the potential distribution via latent variables, the learned embedding. In recent years, several deep generative models are developed such as DeepWalk (Perozzi et al., 2014), Node2vec (Grover & Leskovec, 2016) and GraphGAN (Wang et al., 2018).

3. Proposed Model

In this section, we will show the proposed model, Adaptive Graph Auto-Encoder (AdaGAE) for general data clustering. The core idea is illustrated in Figure 1.

3.1. Probabilistic Perspective of Weighted Graph

Let $p(v|v_i)$ denote connectivity distribution of node v_i . To satisfy the basic property of probability distribution, we have $\sum_{j=1}^n p(v_j|v_i) = 1$.

In general clustering scenario, edges frequently do not exist. Edges and weights need to be constructed via some scheme.

Since $p(v_j|v_i) \geq 0$, the distribution can be viewed as valid weights. Note that $p(v_j|v_i) = p(v_i|v_j)$ has not to hold, and therefore, the constructed graph should be viewed as a directed graph. From this probabilistic perspective, given distances among samples $\{d_{ij}\}_{i,j=1}^n$, we expect that

$$\min_{p(\cdot|v_i)} \sum_{i=1}^n \mathbb{E}_{v_j \sim p(\cdot|v_i)} d_{ij} = \sum_{i=1}^n \sum_{j=1}^n p(v_j|v_i) \cdot d_{ij} \quad (2)$$

so that the constructed graph is locally coherent. However, it is impracticable to solve the above problem directly, as it has a trivial solution: $p(v_i|v_i) = 1$ and $p(v_j|v_i) = 0$ if $j \neq i$. A universal method is to employ *Regularization Loss Minimization*, and the objective can be stated as

$$\min_{p(\cdot|v_i)} \sum_{i=1}^n \mathbb{E}_{v_j \sim p(\cdot|v_i)} d_{ij} + \mathcal{R}(p(\cdot|v_i)) \quad (3)$$

where $\mathcal{R}(\cdot)$ is some regularization term.

In most practical situations, although global distance is usually unreliable, local distance is regarded as a vital part in manifold learning. Similarly, if data is modeled as a graph and the Euclidean distance is used as the measurement of similarities among data points, an ideal distribution should be sparse. More formally, let $\mathbf{p}_i = [p(v_1|v_i), p(v_2|v_i), \dots, p(v_n|v_i)]$ and the sparse distribution should satisfy that $\|\mathbf{p}_i\|_0 \leq \varepsilon$ where ε represents a small constant. Hence, the regularization term should be $\gamma \|\mathbf{p}_i\|_0$. Nevertheless, ℓ_0 -norm is non-convex and it is NP-hard to solve. Generally, we try to solve a convex ℓ_1 relaxation problem, i.e., $\mathcal{R}(p(\cdot|v_i)) = \gamma \|\mathbf{p}_i\|_1$, since ℓ_1 -norm is the tightest convex relaxation of ℓ_0 -norm and it guarantees the sparseness of solution. However, the nondifferentiable problem is hard to optimize and the sparsity degree cannot be controlled. For this problem, we will show that the ℓ_2 -norm relaxation can provide steerable sparsity, which can be solved by analytic solution. To control sparsity of distribution for each node, we utilize point-wise regularization.

Theorem 1. The ℓ_2 -norm relaxation of problem (3)

$$\min_{p(\cdot|v_i)} \sum_{i=1}^n \mathbb{E}_{v_j \sim p(\cdot|v_i)} d_{ij} + \gamma_i \|\mathbf{p}_i\|_2^2 \quad (4)$$

has a k -sparse solution if γ_i satisfies

$$\frac{1}{2}(kd_{i\cdot}^{(k)} - \sum_{v=1}^k d_{i\cdot}^{(v)}) < \gamma_i \leq \frac{1}{2}(kd_{i\cdot}^{(k+1)} - \sum_{v=1}^k d_{i\cdot}^{(v)}) \quad (5)$$

where $d_{i\cdot}^{(v)}$ denotes the v -th smallest value of $\{d_{ij}\}_{j=1}^n$.

The point-wise regularization can control sparsity of each node but also increase the amount of hyper-parameters. In

this paper, we simply choose unified sparsity for all nodes. Formally, γ_i is set as the upper bound

$$\gamma_i = \frac{1}{2}(kd_i^{(k+1)} - \sum_{v=1}^k d_i^{(v)}) \quad (6)$$

It should be emphasized that there is only one hyper-parameter, sparsity k , in our model, which is much easier to tune than the one in traditional ℓ_1 relaxation method. In particular, problem (4) can be solved analytically. The concrete derivation to solve problem (4) and the proof of Theorem 1 will be stated in Section 4.1.

3.2. Graph Auto-Encoder for Weighted Graph

After getting connectivity distribution by solving problem (4), we transfer the directed graph to an undirected graph via $\mathcal{W}_{ij} = (p(v_i|v_j) + p(v_j|v_i))/2$, and the connectivity distribution serves as the reconstruction goal of graph auto-encoder, which will be elaborated soon.

Encoder As shown in (Kipf & Welling, 2017), graphs with self-loop show better performance, i.e., $\tilde{A} = A + I$. Due to $d_{ii} = 0$, $p(v_i|v_i) \in (0, 1)$ if $k > 1$. Moreover, the weight of self-loop is learned adaptively rather than primitive I . Consequently, we can simply set $\tilde{A} = \mathcal{W}$ and $\hat{A} = D^{-\frac{1}{2}} \tilde{A} D^{-\frac{1}{2}}$. The encoder consists of multiple GCN layers and aims to transform raw features to latent features with the constructed graph structure. Specifically speaking, the latent feature is defined as

$$Z = \varphi(\cdots \varphi(\hat{A}XW)) \quad (7)$$

Decoder Instead of reconstructing the weight matrix \tilde{A} , we aim to recover the connectivity distribution $p(v|v_i)$. Firstly, distances of latent features Z are calculated by $\hat{d}_{ij} = \|z_i - z_j\|_2^2$. Secondly, the connectivity distribution is reconstructed by a normalization step

$$q(v_j|v_i) = \frac{e^{-d_{ij}}}{\sum_{j=1}^n e^{-d_{ij}}} \quad (8)$$

The above process can be regarded as inputting $-d_{ij}$ into a softmax layer. Clearly, as d_{ij} is smaller, $q(v_j|v_i)$ is larger. In other words, the similarity is measured by Euclidean distances rather than inner-products used in GAE. To measure difference between two distributions, Kullback-Leibler (KL) Divergence is conventionally utilized. Consequently, the objective function is defined as

$$\begin{aligned} \min_{q(\cdot|v_i)} KL(p||q) &= \sum_{i,j=1}^n p(v_j|v_i) \log \frac{p(v_j|v_i)}{q(v_j|v_i)} \\ \Leftrightarrow \min_{q(\cdot|v_i)} \sum_{i,j=1}^n p(v_j|v_i) \log \frac{1}{q(v_j|v_i)} \end{aligned} \quad (9)$$

Algorithm 1 Algorithm to optimize AdaGAE

Require: Initial sparsity k_0 , upper bound of sparsity k_m and number of iterations to update weight adjacency l .
 $Z = X$, $k = k_0$
for $i = 1, 2, \dots, l$ **do**
 Compute γ_i via Eq. (6).
 Compute $d_{ij} = \|z_i - z_j\|_2^2$.
 Compute $p(\cdot|v_i)$ and \hat{A} by solving problem (4) with k .
 repeat
 Update GAE with Eq. (10) by gradient descent.
 until convergence or exceeding maximum iterations
 Get new embedding Z .
 $k = k + t$
end for
 Perform spectral clustering on \hat{A} .
Ensure: Clustering assignments, weight adjacency \mathcal{W} and embedding Z .

Note that the second line is aiming to minimize the cross entropy, which is widely employed in classification tasks.

Local Structure Preserving A primary drawback of auto-encoder is that there may exist diverse latent representation schemes that can be decoded to the input of encoder due to the powerful representation capacity of neural networks. Nevertheless, some kinds of representations may be useless even harmful. To break this restriction, a popular method is to introduce some prior information such as adversarial auto-encoder (Makhzani et al., 2015) and variational auto-encoder (Kingma & Welling, 2014). Since the similarities are measured by distances and local information is often credible (especially in manifold learning), we add a local structure preserving penalty term into Eq. (9) and thus, the cost function is defined as

$$\begin{aligned} \min_q \sum_{i,j=1}^n p(v_j|v_i) \log \frac{1}{q(v_j|v_i)} + \frac{\lambda}{2} \hat{A}_{ij} \|z_i - z_j\|_2^2 \\ \Leftrightarrow \min_q \sum_{i,j=1}^n p(v_j|v_i) \log \frac{1}{q(v_j|v_i)} + \lambda \text{tr}(Z \hat{L} Z^T) \end{aligned} \quad (10)$$

where $\hat{L} = \hat{D} - \hat{A}$ and λ is a tradeoff parameter to balance cross entropy term and local consistency penalty term.

3.3. Adaptive Graph Auto-Encoder

In last subsection, the weighted adjacency matrix is regarded as fixed during training phase. However, the weighted adjacency matrix is computed through Eq. (4). The whole clustering process should contain connectivity learning and hence, the weighted adjacency should be updated adaptively during training. An intuitive approach is to recompute the

connectivity distribution based on the embedding Z , which contains potential manifold structure information of data. However, the following theorem shows that the simple update based on latent representations may lead to collapse.

Theorem 2. Denote $\hat{d}_{ij} = \|z_i - z_j\|_2$ where z_i is generated by GAE with sparsity k . If $q(\cdot|v_i)$ approximates $p(\cdot|v_j)$ well (numerically) then the solution of

$$\min_{p(\cdot|v_i)} \sum_{i=1}^n \mathbb{E}_{v_j \sim p(\cdot|v_i)} \hat{d}_{ij} + \gamma_i \|p_i\|_2^2 \quad (11)$$

, with the same sparsity, degenerates into an unweighted adjacency matrix.

Intuitively, the unweighted graph is indeed a bad choice for classical clustering tasks. Therefore, the update step with the same sparsity coefficient k may result in collapse. To address this problem, we assume that

Assumption 1. Suppose that the sparse and weighted adjacency is good enough. Specifically, weights of edges are large if it is within a cluster; or small otherwise. Then, under latent representation, samples belonging to the same cluster become more cohesive measured by Euclidean distance.

According to the above assumption, samples from a cluster are more likely to lie in a local area after GAE mapping. Hence, the sparsity coefficient k increases when updating weight sparsity. The step size t which k increases with needs to be discussed. In an ideal situation, we can define the upper bound of k as

$$k_m^* = \min(|C_1|, |C_2|, \dots, |C_c|) \quad (12)$$

where C_i denotes the i -th cluster. Although $|C_i|$ is not known, we can define k_m empirically to ensure $k_m \leq k_m^*$. For instance, k_m can be set as $\lfloor \frac{n}{c} \rfloor$ or $\lfloor \frac{n}{2c} \rfloor$. Accordingly, the step size $t = \frac{k_m - k}{l}$ where l is the number of iterations to update the weight adjacency.

To sum up, Algorithm 1 summarize the whole process of Adaptive Graph Auto-Encoder (AdaGAE).

4. Optimization and Theoretical Analysis

In this section, we first show how to solve problem (4) analytically. Then proofs of the two mentioned theorems are elaborated respectively.

4.1. Optimization of Problem (4)

To keep notations uncluttered, $p(v_j|v_i)$ is simplified as p_{ij} . Then the problem (4) is equivalent to solve the following subproblem individually

$$\min_{p_i^T \mathbf{1}=1, p_i \geq 0} \sum_{j=1}^n p_{ij} d_{ij} + \gamma_i \|p_i\|_2^2 \quad (13)$$

To keep the discussion more concise, the subscript i is neglected. Due to d_j is constant, we have

$$\min_{p^T \mathbf{1}=1, p \geq 0} \sum_{j=1}^n p_j d_j + \gamma \|p\|_2^2 \Leftrightarrow \min_{p^T \mathbf{1}=1, p \geq 0} \|p + \frac{d}{2\gamma}\|_2^2 \quad (14)$$

Then the Lagrangian of the above equation is

$$\mathcal{L} = \|p + \frac{d}{2\gamma}\|_2^2 + \alpha(1 - \sum_{j=1}^n p_j) + \sum_{j=1}^n \beta_j(-p_j) \quad (15)$$

where α and β_j are Lagrangian multipliers. According to KKT conditions,

$$\begin{cases} p_j + \frac{d_j}{2\gamma} - \alpha - \beta_j = 0 \\ \beta_j p_j = 0, \beta_j \geq 0 \\ \sum_{j=1}^n p_j = 1, p_j \geq 0 \end{cases} \quad (16)$$

It is not hard to verify that

$$p_j = (\alpha - \frac{d_j}{2\gamma})_+ \quad (17)$$

where $(\cdot)_+ = \max(\cdot, 0)$. Without loss of generality, suppose that $d_1 \leq d_2 \leq \dots \leq d_n$. According to Theorem 1, $\|p\|_0 = k$, or equivalently, $\alpha - \frac{d_{k+1}}{2\gamma} \leq 0 < \alpha - \frac{d_k}{2\gamma}$ where $k \in [1, n)$. Due to $p^T \mathbf{1} = 1$, we have

$$\alpha = \frac{1}{k} (1 + \sum_{j=1}^k \frac{d_j}{2\gamma}) \quad (18)$$

Substitute Eq. (6) into Eq. (18) and we have

$$p_j = (\frac{d_{k+1} - d_j}{\sum_{j=1}^k (d_{k+1} - d_j)})_+ \quad (19)$$

If $k \geq n$, then it is not hard to verify that Eq. (19) is also the optima. Accordingly, the connectivity distribution can be calculated via close-form solution.

4.2. Proof of Theorem 1

To keep notations uncluttered, we make the same assumption, $d_1 \leq d_2 \leq \dots \leq d_n$.

Proof. To begin with, the auxiliary function

$$f(x) = (1 - \frac{C}{2x})_+, \forall C > 0 \quad (20)$$

is non-decreasing with x . Note that $f(x)$ is strictly increasing when $2x \geq C$. If $\alpha \in [\frac{d_1}{2\gamma}, \frac{d_n}{2\gamma}]$, there must exist m

that satisfies $\alpha - \frac{d_{m+1}}{2\gamma} \leq 0 < \alpha - \frac{d_m}{2\gamma}$. In this case, \mathbf{p} is m -sparse. According to Eq. (18), we have

$$p_j = \frac{1}{m} \left(1 - \frac{\sum_{i=1}^m (d_j - d_i)}{2\gamma} \right)_+ \quad (21)$$

When γ satisfies Eq. (5), we have

$$\frac{1}{m} \left(1 - \frac{\sum_{i=1}^m (d_j - d_i)}{k} \right)_+ \leq p_j \leq \frac{1}{m} \left(1 - \frac{\sum_{i=1}^m (d_j - d_i)}{\sum_{i=1}^k (d_{k+1} - d_i)} \right)_+ \quad (22)$$

according to the non-decreasing property of the auxiliary function $f(x)$. If $m > k$, then

$$0 \leq p_m \leq \frac{1}{m} \left(1 - \frac{\sum_{i=1}^m (d_m - d_i)}{k} \right)_+ \leq 0 \quad (23)$$

Hence, $p_m = 0$ which leads to contradiction. If $m < k$

$$p_{m+1} > \frac{1}{m} \left(1 - \frac{\sum_{i=1}^m (d_{m+1} - d_i)}{\sum_{i=1}^k (d_k - d_i)} \right)_+ > 0 \quad (24)$$

In the first inequality, the equality will never hold due to $2\gamma > \sum_{i=1}^k (d_k - d_i) \geq \sum_{i=1}^k (d_k - d_i)$. Accordingly, \mathbf{p} is at least $(m+1)$ -sparse, which lead to contradiction as well. Therefore, we have $k = m$.

When $(\frac{d_n}{2\gamma}, +\infty)$, it is not hart to verify that $p_m = 0$ which also leads to contradiction. Finally, $\alpha \in (-\infty, \frac{d_1}{2\gamma})$ will never hold due to the constraint $\mathbf{p}^T \mathbf{1} = 1$.

In sum, the theorem is proved. \square

4.3. Analysis of Degeneration

In this part, we will first prove Theorem 2 and then explains the phenomenon from a different perspective. Now, we give the proof of Theorem 2.

Proof. Consider the connectivity distribution of v_1 and suppose that $p(v_1|v_1) \geq p(v_2|v_1) \geq \dots \geq p(v_k|v_1) > 0 = p(v_{k+1}|v_1) = \dots = p(v_n|v_1)$. When $KL(p||q)$ approximates 0 numerically, we have

$$\hat{d}_{1i} \ll \hat{d}_{1j}, \forall i \leq k, j > k \quad (25)$$

If we update \hat{A} by Eq. (19) based on $\{\hat{d}_{ij}\}_{i,j=1}^n$, then for any $i \leq k$,

$$p(v_i|v_1) = \frac{\hat{d}_{1,k+1} - \hat{d}_{1i}}{\sum_{j=1}^k (\hat{d}_{1,k+1} - \hat{d}_{1i})} \rightarrow \frac{1}{k} \quad (26)$$

due to $\forall i \leq k, \hat{d}_{1i} \ll \hat{d}_{1,k+1}$. The proof is easy to extend to other nodes. Hence, the theorem is proved. \square

On the other hand, the following theorem demonstrates that the SoftMax output layer with $-\hat{d}_{ij}$ is equivalent to solve problem (3) with a totally different regularization. Therefore, the perfect approximation may lead to bad performance.

Theorem 3. *The decoder of AdaGAE is equivalent to solve the following problem*

$$\min_{q(\cdot|v_i)} \sum_{i=1}^n \mathbb{E}_{v_j \sim q(\cdot|v_i)} \hat{d}_{ij} - H_i(v) \quad (27)$$

where $H_i(v) = -\sum_{j=1}^n q(v_j|v_i) \log q(v_j|v_i)$ represents the entropy of connectivity distribution of node v_i .

The proof is stated in supplementary material.

4.4. Spectral Analysis

As mentioned in subsection 3.2, AdaGAE generates a weighted graph with adaptive self-loops. Analogous to SGC (Wu et al., 2019), adaptive self-loops also reduce the spectrum of normalized Laplacian. Formally,

Theorem 4. *Let $\hat{A}' = A - \text{diag}(\hat{A})$ and $\tilde{A}' = \hat{D}'^{-\frac{1}{2}} \hat{A}' \hat{D}'^{-\frac{1}{2}}$. According to eigenvalue decomposition, suppose $I - \tilde{A} = Q\Lambda Q^T$ and $I - \tilde{A}' = Q'\Lambda'Q'^T$. The following inequality always holds*

$$0 = \lambda_1 = \lambda'_1 < \lambda_n < \lambda'_n \quad (28)$$

The proof is stated in supplementary material. This theorem indicates the adaptive self-loops smooth the Laplacian matrix as well.

5. Experiments

In this section, details of AdaGAE are demonstrated and the results are shown. The visualization supports theoretical analysis mentioned in the last section.

5.1. Datasets

AdaGAE are evaluated on totally 7 datasets, including UMIST (Hou et al., 2013), JAFFE (Lyons et al., 1999), ORL (Cai et al., 2010), PALM, COIL20 (Nene et al., 1996), YALE (Georghiades et al., 2001) and USPS (Hull, 1994). The concrete information is summarized in Table 3. All features are rescaled to $[0, 1]$. As how to apply GCN on large graph is still a challenging problem and it is not the focus of this paper, we only conduct experiments on small and middle scale datasets. A feasible method is to replace the encoder with GCN designed for large scale datasets, such as StoGCN (Chen et al., 2018), Cluster-GCN (Chiang et al., 2019), etc.

Table 1. ACC (%)

Methods	UMIST	JAFFE	ORL	PALM	COIL20	YALE	USPS
SC	29.01	70.14	56.43	19.54	56.42	29.58	28.75
K-Means	42.87	72.39	54.75	70.39	58.26	41.33	64.67
FKSC	50.64	79.58	69.33	75.30	69.78	50.96	64.05
CAN	69.62	96.71	68.00	88.10	84.10	49.09	67.96
DFKM	45.47	90.83	61.43	67.45	60.21	51.43	73.42
DEC	36.47	62.95	27.45	74.35	50.42	42.30	71.22
GAE (fixed \tilde{A})	73.22	96.71	71.75	88.30	92.43	57.58	67.48
AdaGAE (fixed sparsity)	32.00	47.42	68.00	91.80	33.82	57.58	34.09
AdaGAE	83.48	97.27	71.40	95.25	93.75	57.58	91.96

Table 2. NMI (%)

Methods	UMIST	JAFFE	ORL	PALM	COIL20	YALE	USPS
SC	30.77	77.94	75.69	37.25	71.06	34.78	21.54
K-Means	65.47	80.90	75.43	89.98	74.58	48.71	62.88
FKSC	67.67	84.24	83.32	93.28	80.75	50.38	65.83
CAN	87.75	96.39	83.58	97.08	90.93	56.18	78.85
DFKM	67.04	92.01	81.13	86.74	76.81	55.92	71.58
DEC	56.96	82.83	55.22	90.37	69.43	48.71	72.25
GAE (fixed \tilde{A})	87.04	96.39	84.51	96.96	97.26	76.93	76.45
AdaGAE (fixed sparsity)	52.08	59.55	83.65	97.80	55.46	76.93	35.39
AdaGAE	91.03	96.78	85.34	98.18	98.36	76.93	84.81

Table 3. Information of Datasets

Name	# Features	# Size	# Classes
UMIST	1024	575	20
JAFFE	1024	213	10
ORL	1024	400	40
PALM	256	2000	100
COIL20	1024	1440	20
YALE	1024	165	15
USPS	256	9298	10

5.2. Compared Methods

To evaluate AdaGAE, totally 6 methods are compared, including Spectral Clustering (SC) (Ng et al., 2002), K-Means, FKSC (Zhang et al., 2018), CAN (Nie et al., 2014), DFKM (Zhang et al., 2019) and DEC (Xie et al., 2016). Roughly speaking, SC, K-Means, FKSC and CAN are traditional clustering approaches while DFKM and DEC are deep clustering models with different embedded clustering models. Hyper-parameters of these methods are searched via the same pattern recorded in the corresponding papers. Codes of these methods are downloaded from homepages of authors.

5.3. Experimental Setup

In our experiments, the encoder consists of two GCN layers. If the input dimension is 1024, the first layer has 256 neurons and the second layer has 64 neurons. Otherwise, the two layers have 128 neurons and 64 neurons respectively. The activation function of the first layer is set as ReLU while the other one employs linear function. The initial sparsity k is set as 5 and the upper bound k_m is searched from $\{\lfloor \frac{n}{c} \rfloor, \lfloor \frac{n}{2c} \rfloor\}$. The tradeoff coefficient λ is searched from $\{10^{-3}, 10^{-2}, \dots, 10^3\}$. The number of graph update step is set as 10 and the maximum iterations to optimize GAE varies in [50, 100].

To verify the effect of the adaptive process, two extra experiments are conducted: GAE with fixed \tilde{A} and AdaGAE with fixed sparsity k . Note that all hyper-parameters are same except for the specific setting.

Two popular clustering metrics, accuracy (ACC) and normalized mutual information (NMI), are employed to evaluate performance. All methods are run 10 times and the means are reported. The code is implemented under pytorch-1.3.1 on a Windows 10 PC with a NVIDIA GeForce GTX 1660 GPU and 8 i7 cores. The exact values of hyper-parameters can be found in supplementary material.

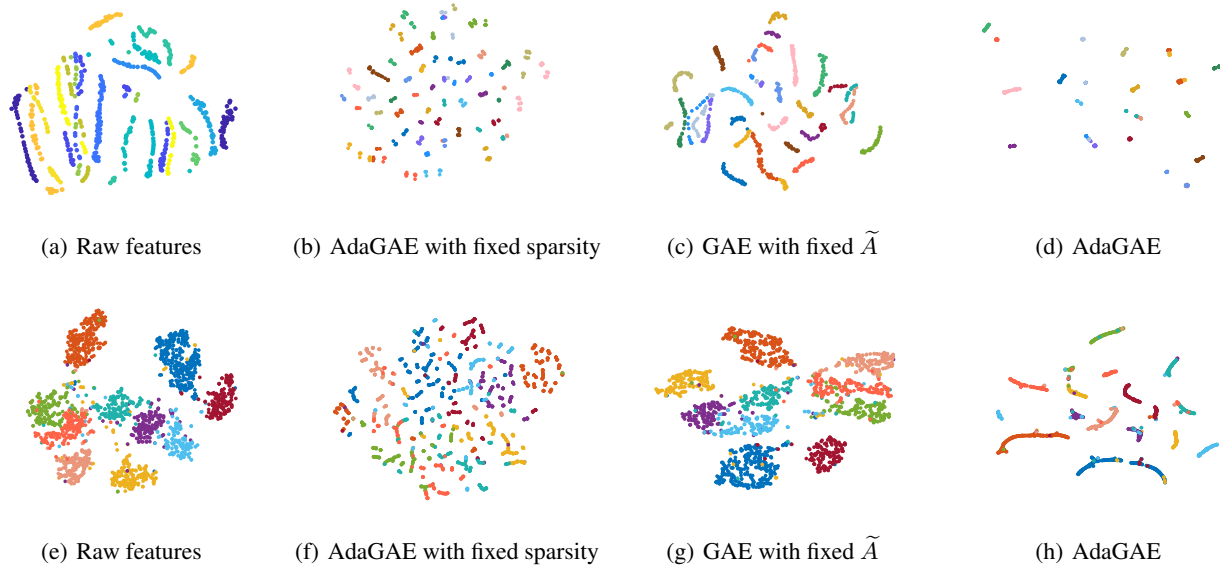


Figure 2. t-SNE visualization on UMIST and USPS: The first line illustrates results on UMIST and the second line shows results on USPS. Clearly, AdaGAE projects semblable samples into the same embedding. Notice that a few data points are projected into wrong group which are usually regarded as outliers.

5.4. Experimental Results

ACC and NMI of all mentioned methods are summarized in Table 1 and Table 2, respectively. The best results of both competitors and AdaGAEs are highlighted in boldface. From Table 1 and Table 2, we conclude that:

- Classical deep clustering models suffer from overfitting and work poorly on small scale datasets while AdaGAE is stable on all datasets. Moreover, the improvement caused by graph convolution is impressive. Specifically, AdaGAE outperform DFKM about 20% on ACC and 7% on NMI for USPS.
- When the sparsity k keeps fixed, AdaGAE collapses on UMIST, JAFFE, COIL20 and USPS. For example, ACC shrinks about 50% and NMI shrinks about on COIL20.
- From the comparison of two extra experiments, we confirm that the adaptive graph update process plays a positive role on most datasets except for ORL, which may be caused by too few samples in each cluster such that it is hard to define k and k_m .

Besides, Figure 2 illustrates the learned embedding vividly. Combining with Theorem 2, if k is fixed as a constant, then \hat{A} degenerates into an unweighted adjacency matrix and a cluster is broken into a mass of groups. Each group only contains a small amount of data points and they scatter

chaotically which leads to collapse. Instead, the adaptive process introduced in Section 3.3 connects these groups before degeneration via increasing sparsity k and hence, the embeddings in a cluster become pretty cohesive. It should be emphasized that a large k_0 frequently leads to capture wrong information. After transformation of GAE, the nearest neighbors are more likely to belong with a same cluster and thus it is rational to increasing k_0 with an adequate step size.

6. Conclusion

In this paper, we propose a novel clustering model for general data clustering, namely Adaptive Graph AutoEncoder (AdaGAE). Generative graph representation model is utilized to construct a weighted graph with steerable sparsity. To exploit potential information of data, we employ graph convolution operator and thus a graph auto-encoder with local structure preserving is designed. More importantly, as the graph used in GAE is constructed artificially, an adaptive update step is developed to update graph with the help of learned embedding. Related theoretical analysis demonstrates the reason why AdaGAE with fixed sparsity collapses in update step. In experiments, we verify the effectiveness of adaptive update step by removing the corresponding part of AdaGAE. Surprisingly, the visualization supports the theoretical analysis well and confirms the necessary of the adaptive graph update.

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A. Proof of Theorem 3

Proof. Problem (27) is equivalent to the following i -th sub-problem

$$\begin{aligned} \min_{q_{ij}} \quad & \sum_{j=1}^n q_{ij} \hat{d}_{ij} + q_{ij} \log q_{ij} \\ \text{s.t.} \quad & \sum_{j=1}^n q_{ij} = 1, q_{ij} > 0 \end{aligned} \quad (29)$$

Similarly, the subscript i is omitted to keep notations uncluttered. The Lagrangian is

$$\mathcal{L} = \sum_{j=1}^n q_j \hat{d}_j + q_j \log q_j + \alpha(1 - \sum_{j=1}^n q_j) + \sum_{j=1}^n \beta_j(-q_j) \quad (30)$$

Then the KKT conditions are

$$\begin{cases} \hat{d}_j + 1 + \log q_j - \alpha - \beta_j = 0 \\ 1 - \sum_{j=1}^n q_j = 0 \\ \beta_j q_j = 0 \\ \beta_j \geq 0 \end{cases} \quad (31)$$

Due to $q_j > 0$, $\beta_j = 0$. Use the first line, we have

$$q_j = \exp(\alpha - \hat{d}_j - 1) \quad (32)$$

Combine it with the second line and we have

$$\exp(\alpha) \sum_{j=1}^n \exp(-\hat{d}_j - 1) = 1 \quad (33)$$

Furthermore, we have

$$q_j = \frac{\exp(-\hat{d}_j - 1)}{\sum_{j=1}^n \exp(-\hat{d}_j - 1)} = \frac{\exp(-\hat{d}_j)}{\sum_{j=1}^n \exp(-\hat{d}_j)} \quad (34)$$

With $\hat{d}_{ij} = \|z_i - z_j\|_2$, the theorem is proved. \square

B. Proof of Theorem 4

It should be pointed out that the proof imitates the corresponding proof in (Wu et al., 2019). Analogous to Lemma 3 in (Wu et al., 2019), we first give the following lemma without proof,

Lemma 1. Let $\alpha_1 \leq \alpha_2 \leq \dots \leq \alpha_n$ be eigenvalues of $\hat{D}^{-\frac{1}{2}} \hat{A}' \hat{D}^{-\frac{1}{2}}$ and $\beta_1 \leq \beta_2 \leq \dots \leq \beta_n$ be eigenvalues of $\hat{D}'^{-\frac{1}{2}} \hat{A}' \hat{D}'^{-\frac{1}{2}}$. The following inequality always holds

$$\alpha_1 \geq \frac{\beta_1}{1 + \min \frac{\hat{A}_{ii}}{\hat{D}'_{ii}}}, \alpha_n \leq \frac{1}{1 + \max \frac{\hat{A}_{ii}}{\hat{D}'_{ii}}} \quad (35)$$

Dataset	λ	k_0	γ	t_i	k_m	t
UMIST	1	5	10^{-3}	50	$\lfloor \frac{n}{c} \rfloor$	10
COIL20	1	5	10^{-2}	100	$\lfloor \frac{n}{2c} \rfloor$	10
JAFFE	10^{-3}	5	10^{-2}	20	$\lfloor \frac{n}{c} \rfloor$	10
PALM	10	10	10^{-3}	50	$\lfloor \frac{n}{c} \rfloor$	10
YALE	2^9	5	10^{-1}	150	$\lfloor \frac{n}{c} \rfloor$	10
ORL	1	5	5×10^{-3}	150	$\lfloor \frac{n}{2c} \rfloor$	10
USPS	10^{-2}	5	5×10^{-3}	150	$\lfloor \frac{n}{c} \rfloor$	10

Table 4. λ : local information, k_0 : initial sparsity, γ : learning rate, λ : regularization coefficient, t_i : number of iterations to update GAE

For all datasets, we simply rescale features into $[0, 1]$. All datasets are downloaded from <http://www.esience.cn/people/fpnle/index.html>.

The proof is apparent according to Lemma 3 provided in (Wu et al., 2019). The proof is given as follows

Proof. Let $M = \text{diag}(\hat{A})$ and we have

$$\begin{aligned}
 \lambda_n &= \max_{\|\mathbf{x}\|=1} \mathbf{x}^T (I - \hat{D}^{-\frac{1}{2}} M \hat{D}^{-\frac{1}{2}} - \hat{D}^{-\frac{1}{2}} \hat{A}' \hat{D}^{-\frac{1}{2}}) \mathbf{x} \\
 &\leq 1 - \min \frac{\hat{A}_{ii}}{\hat{D}'_{ii} + \hat{A}_{ii}} - \alpha_1 \\
 &\leq 1 - \min \frac{\hat{A}_{ii}}{\hat{D}'_{ii} + \hat{A}_{ii}} - \frac{\beta_1}{1 + \min \frac{\hat{A}_{ii}}{\hat{D}'_{ii}}} \\
 &\leq 1 - \frac{\beta_1}{1 + \min \frac{\hat{A}_{ii}}{\hat{D}'_{ii}}} \\
 &\leq 1 - \beta = \lambda'_n
 \end{aligned}$$

□

C. Experimental Details

The exact values of AdaGAE in our experiments are reported in Table 4. To use SC, we construct the graph via Gaussian kernel, which is given as

$$w_{ij} = \frac{\exp(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2}{\sigma})}{\sum_{j \in \mathcal{N}_i} \exp(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2}{\sigma})} \quad (36)$$

where \mathcal{N}_i represents m -nearest neighbors of sample \mathbf{x}_i . m is searched from $\{5, 10\}$ and σ is searched from $\{10^{-3}, 10^{-2}, \dots, 10^3\}$.

The maximum iterations of GAE with fixed \tilde{A} is set as 200. Note that its objective function is defined as Eq. (10).

Codes of K-means, SC, FKSC, and CAN are implemented under MATLAB 2019a, while codes of DFKM, DEC and AdaGAE are implemented under python 3.6.