Differential equation and probability inspired graph neural networks for latent variable learning

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Abstract—Probabilistic theory and differential equation are powerful tools for the interpretability and guidance of the design of machine learning models, especially for illuminating the mathematical motivation of learning latent variable from observation. Subspace learning maps high-dimensional features on low-dimensional subspace to capture efficient representation. Graphs are widely applied for modeling latent variable learning problems, and graph neural networks implement deep learning architectures on graphs. Inspired by probabilistic theory and differential equations, this paper conducts notes and proposals about graph neural networks to solve subspace learning problems by variational inference and differential equation. Source code of this paper is available at https://github.com/zshicode/Latent-variable-GNN.

Index Terms—Subspace learning, differential equations, graph neural networks, latent variable learning, variational inference

I. INTRODUCTION

LATENT variable learning consists of algorithms that predict latent variable from observation. The subspace learning problem is defined from the motivation that predict latent variable from observation. The observed features $X$ are usually high-dimensional, yet machine learning models perform much better on analyzing low-dimensional representations. The latent representations span the low-dimensional subspace. The subspace may follow some constraints, usually low-rank constraints, sparse constraints and manifold constraints. Such constraints can be modeled through numerical
optimization programming, but usually with probabilistic theory and differential equation as well. Appendix summarizes some classical subspace learning methods.

Subspace learning usually conducts manifold constraint. Manifold constraint is motivated by the manifold in differential geometry, which can derive some remarkable partial differential equations (PDE). The Laplacian operator in PDE is correspond to the Laplacian matrix of a matrices. This idea can derive a series of ordinary differential equations (ODE) to describe the Laplacian-participated linear dynamic systems. Label propagation [31], [32], [39] follows manifold regularization [3]. For semi-supervised iterative algorithms such as label propagation algorithm and pagerank, establishing the equivalent relationship between its iterative equation and deep learning network can improve the effect of label propagation algorithm, and design semi-supervised iterative algorithms in deep learning network.

Graph neural networks [14], [24] (GNN) is widely applied to model graph relationship for deep learning [12], [13], [27]. Graphs are widely applied for modeling latent variable learning problems, and graph neural networks implement deep learning architectures on graphs.

Vanilla GNN focus on classification task upon nodes on a graph. The graph convolutional networks (GCN) [14], GraphSAGE [11], MPNN (message passing network) [10], graph attention networks (GAT) [30], graph autoencoders (GAE) [15], variational graph autoencoders (VGAE) [15], attention-based graph neural networks (AGNN) [28], graph isomorphism network (GIN) [36] and many other models were proposed. Subspace learning and differential equation guided graph neural networks [17], [33] are useful for detecting subspace with low-rank or sparse property, or with better manifold smoothness. Probabilistic theory inspired graph neural networks [15], [27], such as variational inference and conditional random field, are powerful for detecting latent variable dependency and learning efficient representation.

II. DIFFERENTIAL EQUATION AND PROBABILITY INSPIRED GRAPH NEURAL NETWORKS

A. ODE inspired graph neural networks

Deep learning and differential equations (dynamic systems) have certain equivalence under certain conditions. For example, ResNet can be regarded as the form of solving the optimal control problem. The process of network training can be regarded as the form of solving the optimal control problem and feedback form of the differential equation, the process of network training can be the form of an iterative equation. For example, the GCN in [14] can be written as (transductive learning)

\[
\mathbf{h}^{(k)}(x) \leftarrow \frac{1}{d_i + 1} \mathbf{h}^{(k-1)}(x) + \sum_{j=1}^{n} \frac{1}{(d_j + 1)(d_j + 1)} \mathbf{h}^{(k-1)}(j),
\]

GraphSAGE [11] can be written as (inductive learning)

\[
\bar{\mathbf{h}}^{(k)}(x) \leftarrow \frac{1}{d_i + 1} \left( \mathbf{h}^{(k-1)}(x) + \sum_{j=1}^{n} \mathbf{h}^{(k-1)}(j) \right),
\]

PageRank [21] can be written as

\[
h_u = \frac{1 - \alpha}{N} + \alpha \sum_{v \in N(u)} h_v
\]

Among them, \(\alpha\) is called the damping factor, which is generally taken as 0.85, \(N\) is the number of nodes in the entire graph, and \(d_i\) represents the degree of the node, which is similar to the message passing mechanism of GCN.

Consider the one-dimensional Weisfeiler-Lehman (WL-1) algorithm

\[
h_i^{(t+1)} \leftrightarrow \text{hash} \left( \sum_{j \in N_i} h_j^{(t)} \right)
\]

Here \(h_i^{(t)}\) represents the "color" (i.e. label information) of the node \(v_i\) at the \(t\)th iteration, and \(N_i\) represents its neighborhood. Replace the hash operation with a neural network, then

\[
h_i^{(t+1)} = \sigma \left( \sum_{j \in N_i} \frac{1}{d_{ij}} W_j^{(t)} \right)
\]

The discrete iteration is linked to dynamic programming. [37] considered graph neural networks with the relaxation step of Bellman-Ford algorithm.

\[
d[t + 1][s] = \min_{j \in N_i} [d[t][j] + w[j][s]]
\]

Inspired by the Neural ODE [7], [34] proposes a continuous graph neural network (continuous GNN), and uses the ordinary differential equation model to explain the GNN.

B. PDE inspired graph neural networks

1) Heat conduction equation inspiration: Use \(\Delta\) to represent the Laplacian operator (harmonic operator), such as in the two-dimensional case

\[
\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}
\]

Use \(\Delta^2\) for the biharmonic operator, e.g. in the two-dimensional case

\[
\Delta^2 = \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right)^2 = \frac{\partial^4}{\partial x^4} + 2 \frac{\partial^4}{\partial x^2 \partial y^2} + \frac{\partial^4}{\partial y^4}
\]

On the graph \(\Delta\) represents the normalized Laplacian matrix (the Laplacian operator on the discretized manifold), and the biharmonic operator \(\Delta^2 \approx \Delta^T \Delta\).

**Theorem 1.** The following equality holds that

\[
\min y^T \Delta y \Leftrightarrow \min \|\nabla y\|^2
\]
Proposition 1. First-order CRF is linked to $\min y^T\Delta y$, second order is linked to $y^T\Delta^2 y$. (See Theorem 13 and 15)

Now generalize (10) to the graph.

Definition 2 (Heat conduction equation on graph). For the heat $u_i$ of node $i$ we have

$$\Delta u_i = \sum_{j \in N(i)} w_{ij} u_j - d_i u_i$$

so

$$\Delta u = (W - D)u = -Lu$$

so

$$\partial u/\partial t = -Lu$$

Heat distribution $K_t = \exp(-tL)$, where $K_t(i, j)$ represents the heat conducted from $i$ to $j$ at time $t$. Kernel $K_t$ is equivalent to setting edge weights as $\exp(-tL)$.

Theorem 2. The biharmonic operator is equivalent to minimizing $\|\Delta y\|^2$.

Proposition 2. (40) suggests that the semi-supervised learning problem on the graph is equivalent to solving the harmonic equation $\Delta y = 0$, and the boundary condition is the label of the marked point, which is equivalent to minimizing $y^T\Delta y$.

2) PDE inspired spectral GNN:

Proposition 3. Green function of (17)

$$G = \int_0^{+\infty} K_t dt = L^{-1}$$

After introducing Green function, $y_u$ can be calculated like this

$$y_u = G_{uu}W_u y_i$$

which is

$$f(j) = \sum_{i=1}^n \sum_{k \in \mathcal{N}(j)} y_i w_{ik} G(k, j)$$

This is how to write $f$ as a kernel classifier.

Definition 3 (Heat kernel). The solution to the equation (17) is

$$K_t(x, 0) = K_t(x) = \int_0^\infty \kappa_t(x, y) f(y) dy$$

Where $\kappa_t$ is called the heat kernel, and heat kernel has the following properties:

$$\kappa_t(x, y) = \sum_{i=1}^{+\infty} e^{-\lambda_i t} u_i^T(x) u_i(y)$$

where $i$ is the $i$-th eigenvector of the Laplacian matrix.

In addition, the spectrum of $K_t = \exp(-tL)$ can also be studied, and if $\lambda_i$ represents the eigenvalue of $L$, this group of basis $e^{-\lambda_i t}$ can be investigated. In the frequency domain, that is, a set of basis $e^{-\lambda_i t}$, which is the idea of Fourier transform. In fact, the Fourier transform is derived from the solution of the heat conduction equation.

Proposition 4. Note that the first-order Taylor expansion of $e^{-\lambda_i t}$ is $1 - \lambda_i t$, so it can be considered that $e^{-\lambda_i t} \approx (1 - \lambda_i t)$, while $(1 - \lambda)^k$ corresponds to the $k$ order filter in the graph convolution.
Message passing process in the graph neural network can also be regarded as a process of "heat" propagation, and it can also be regarded as a kind of label propagation. \cite{24} is very similar to the Fourier transform on a graph. And Fourier transform on the graph is closely related to the graph neural network.

3) PDE inspired spatial GNN: Above, we have proposed an understanding of the graph neural network method in the spectral domain.

For the graph neural network method in the spatial domain, for example, AGNN \cite{25} calculates $e_{ij} = \beta \cos(z_i, z_j)$. Where $\beta \in (0, 1)$ is a learnable parameter, and then do softmax to get the weight

$$w_{ij} = \frac{\exp e_{ij}}{\sum_{k \in N(i)} \exp e_{ik}} \tag{25}$$

This is very similar to the RBF kernel because

$$e_{ij} = -\frac{\|z_i - z_j\|^2}{2\sigma^2} = -\frac{2(1 - \cos(z_i, z_j))}{2\sigma^2} \tag{26}$$

This is using the attention mechanism to learn edge weights similar to RBF.

C. On Laplacian matrix

The original Laplacian matrix

$$\mathcal{L} = D - A \tag{27}$$

In graph signal processing \cite{33}, graph filtering problems often correspond to the following optimization problems

$$\min_x x^T \mathcal{L} x \quad \text{s.t. } x^T D x = \text{trace} D \tag{28}$$

in

$$x^T \mathcal{L} x = \frac{1}{2} \sum_{i,j} a_{ij} (x_i - x_j)^2 \tag{29}$$

is called the total variation operator, the Lagrange multiplier of the above optimization problem is

$$x^T \mathcal{L} x - \lambda (x^T D x - \text{trace} D) \tag{30}$$

So the solution is the generalized eigenvalue problem as follows

$$\mathcal{L} x = \lambda D x \iff \mathcal{L}^{-1} x = \lambda x \tag{31}$$

Its generalized Rayleigh entropy is

$$R = \frac{x^T \mathcal{L} x}{x^T D x} \tag{32}$$

Let $y = D^{1/2} x$ then

$$R = \frac{y^T D^{-1/2} \mathcal{L} D^{-1/2} y}{y^T y} \tag{33}$$

This leads to two forms of regularized Laplacian matrix, one of which is the symmetric regularized Laplacian matrix

$$L = D^{-1/2} \mathcal{L} D^{-1/2} = I - D^{-1/2} AD^{-1/2} \tag{34}$$

The second is the regularized Laplacian matrix of the random walk

$$L_{rw} = D^{-1} \mathcal{L} = I - D^{-1} A \tag{35}$$

Note that $D^{-1} A$ is exactly the state transition matrix of the random walk (this Markov process). $D^{-1} A$ is similar to $D^{-1/2} AD^{-1/2}$ and has the same eigenvalues, if $v$ is $D^{-1} A$, then $D^{1/2} v$ is the eigenvector of the eigenvalue corresponding to $D^{-1/2} AD^{-1/2}$.

Theorem 4 (Spectral radius of non-negative matrix). For a non-negative matrix $A$ of order $n$:

$$\min_i \sum_j a_{ij} \leq \rho(A) \leq \max_j \sum_i a_{ij} \tag{36}$$

Theorem 5 (Perron-Frobenius). If $A$ is a non-negative matrix of order $n$, then:

- $\rho(A) > 0$, and the algebraic multiplicity of the eigenvalue corresponding to $\rho(A)$ is 1;
- There is a unique vector $x$ such that $Ax = \rho(A)x$, and $x_i > 0$, $\sum_i x_i = 1$, called the right Perron vector;
- There is a unique vector $y$ such that $y^T A = \rho(A)y^T$, and $y_i > 0$, $\sum_i y_i = 1$, called the left Perron vector;
- If $A$ is a positive matrix, then the geometric multiplicity of the eigenvalue corresponding to $\rho(A)$ is 1, and

$$\lim_{m \to \infty} (\rho(A)^{-1} A)^m = xy^T \tag{38}$$

Theorem 6 (Eigenvalues of the regularized Laplacian matrix). The eigenvalues of the regularized Laplacian matrix lie in the interval $[0, 2]$, and for any graph (the number of nodes is not less than 2), $L$ has an eigenvalue of 0, only for bipartite graphs, $L$ has an eigenvalue of 2.

\cite{17} used the above properties to explain the over-fitting problem of GCN, and proposed a method for co-training and self-training of GCN to avoid over-fitting. Regardless of the activation function, the one-step iteration formula of GCN is $H = \hat{A}X\Theta$, so multi-layer GCN can be written as

$$Z = \hat{A} \cdots \hat{A}X\Theta_1 \cdots \Theta_k = \hat{A}^k X\Theta_1 \cdots \Theta_k \tag{39}$$

Let $\hat{A} = D^{-1} A$, since $\rho(\hat{A}) = 1$, so

$$\lim_{k \to \infty} \hat{A}^k = \begin{pmatrix} 1/\sqrt{n} \\ \vdots \\ 1/\sqrt{n} \end{pmatrix} \cdot \begin{pmatrix} 1/\sqrt{n}, \cdots, 1/\sqrt{n} \end{pmatrix} = \frac{1}{n} E \tag{40}$$

where $E$ represents an all-one matrix. This means that in a deep GCN, if no improvement is made, the features are equivalent to propagating on a (including self-loop) fully connected graph. After neighborhood aggregation, the features at all points converge, making the GCN classification ability significantly reduced.

Proposition 5. The optimal number of layers $k$ of GCN satisfies

$$d^k n_l = n \tag{41}$$
Where $\bar{d}$ represents the average degree of nodes, $n_1, n$ represent the number of marked nodes and the total number of nodes, respectively. This means that after $k$ layers of GCN, the features on the marked nodes can just be transferred to the full graph. [17]

The following considers adding a self-loop to the graph, $\hat{A} = A + \gamma I$, (generally $\gamma = 1$), [33]. These discussions are for undirected unweighted graphs (i.e., the adjacency matrix is symmetric 0-1 matrix).

**Proposition 6.** Adding a self-loop to the graph can reduce the maximum eigenvalue of the regularized Laplacian matrix.

**Theorem 7.** Conjecture that the

$$\hat{\lambda}_n = 1 - \frac{\gamma}{\gamma + \bar{d}} - \frac{\bar{d}}{\gamma + \bar{d}} \beta_1$$

As an estimate of $\hat{\lambda}_n$, $-1 < \beta_1 < 0$ and generally $\beta_1 \approx -1$,

so

$$\hat{\lambda}_n \approx 1 - \frac{\gamma}{\gamma + \bar{d}} + \frac{\bar{d}}{\gamma + \bar{d}} = \frac{2\bar{d}}{\gamma + \bar{d}}$$

This approximation can significantly reduce the amount of computation for $\hat{\lambda}_n$, in fact, $\bar{d}$ is the quotient of the total number of edges divided by the total number of nodes, in other words, the sum of adjacency matrix elements divided by the matrix order 's business.

**D. Graph neural networks inspired by differential equation**

1) **Label propagation and manifold learning:** A graph is the discretized form of a manifold, thus $f$ can also be regarded as the discretized form of $f$, with its values equivalent to the values of $f$ at the nodes of the graph. In such a viewpoint, the matrix I-W can be regarded as the graph Laplacian of this pasted graph intuitively. $L$ is the Laplacian-Beltrami operator defined on the data manifold, and $f$ is the function defined on this manifold.

**Proposition 7.** Semi-supervised learning problem on the graph is equivalent to solving the harmonic equation $\Delta f = 0$, and the boundary condition is the label of the marked point, which is equivalent to minimizing $f^T \Delta f$. Minimizing $f^T \Delta f$ is equivalent to minimizing $\|\nabla f\|^2$.

**Proposition 8.** Use $L$ to represent the regularized Laplacian matrix, in the spectral clustering [29], convert the solution equation $L f = 0$ (that is, find the eigenvector of $L$) to minimize $f^T L f$, and solving such an eigenvalue decomposition problem is equivalent to finding an optimal solution to a graph cut problem (i.e., normalized cut).

**Proposition 9.** Relax the solution equation $L f = 0$ (that is, find the eigenvector of $L$) to minimize $\|L f\|^2 = f^T L^2 f$, that is, solve the equation $L^T L f = 0$, that is, the biharmonic equation $\Delta^2 f = 0$.

Label propagation can be regarded as a Laplacian least square method [3], and its optimization objective is

$$\min_F F^T L F + \frac{\gamma}{2} \|F - Y\|_F^2$$

Considering that the regularized Laplace matrix can be written as $L = I - W$, where $W$ is the normalized edge weight, the optimal solution is $F^* = (1 - \alpha)(I - \alpha W)^{-1}Y$, here $\alpha = 1/(1 + \gamma)$. This can be obtained by iterating $F(k) = \alpha W F(k-1) + (1 - \alpha)Y$, $0 < (1 - \alpha) \ll 1$. Let $\eta = 2/\gamma$,

$$\min_F \eta \text{tr}(F^T LF) + \|YF\|^2$$

$$\Rightarrow \eta LF + YF = 0$$

$$\Rightarrow F = (I + \eta L)^{-1}Y$$

And when the spectral radius of $\eta L$ is not greater than 1, the first-order Taylor expansions of $(I + \eta L)^{-1}$ and $e^{-\eta L}$ are both $I - \eta L$. Use $F = W(W + \eta LW)^{-1}Y$ to find $F$ [35], where $\eta$ is a hyperparameter, then

$$F = W(W + \eta LW)^{-1}Y$$

$$= W(W^{-1} - W^{-1}(\eta L)(I + \eta L)^{-1})Y$$

$$= (I - \eta L(I + \eta L)^{-1})Y$$

$$= (I + \eta L)^{-1}Y$$

In this paper, when using GCN for node classification, the iterative form of GCN is

$$H_{k+1} = (I + \eta L)^{-1}H_k \Theta_k, \eta > 1$$

It is propagated according to the label. The formula $F = (I + \eta L)^{-1}Y$ improves the practice of GCN. This paper sets $\eta = 2$. The label propagation parameter $\eta$ selection in POGNN is on Appendix.

**Theorem 8.** The graph filtering that combines graph convolution and label propagation [17], suggests that label propagation algorithm is an optimization problem

$$\min_Z \|Z - Y\|^2 + \alpha \text{trace}(Z^T LZ)$$

so

$$Z = (I + \alpha L)^{-1}Y$$

where $L$ is the (normalized) Laplacian matrix and $Y$ is the label.

Remark of this Theorem is on Appendix.

2) **Edge weight computation inspired by differential equation:** The label propagation algorithm is similar in form to the graph neural network. The edge weight of the label propagation algorithm is determined according to the distance between the features. The goal is to make the weight between the similar feature points as large as possible. In the graph neural network, the weight of the edge is set according to the actual problem, or learn it with the attention mechanism. e.g. [30] setting

$$z_i^{(l)} = \Theta^{(l)} h_i^{(l)}$$

$$e_{ij}^{(l)} = \text{LeakyReLU}(\alpha^{(l)}(z_i^{(l)} / \|z_i^{(l)}\|)$$

$$w_{ij}^{(l)} = \exp(e_{ij}^{(l)}) / \sum_{k \in N(i)} \exp(e_{ik}^{(l)})$$

$$h_i^{(l+1)} = \sigma \left( \sum_{j \in N(i)} w_{ij}^{(l)} z_j^{(l)} \right)$$

(48)
where $\Theta, \alpha$ is the parameter learned by the neural network.

AGNN \cite{28} uses the process of calculating the above $e_{ij}$ to be replaced by cosine similarity, $e_{ij} = \beta \cos(z_i, z_j)$, where $\beta \in (0, 1)$ is a learnable parameter. MPNN (message passing network) \cite{10} uses a fully connected layer to map the feature vector of the source node to the edge weight, i.e. passing network [10] uses a fully connected layer to map the feature vector of the source node to the edge weight, i.e. $w_{ij} = FFN(N(z_j))$.

The label propagation algorithm can be regarded as the idea of manifold learning and ODE. The RBF and neural network based edge weights computation is also inspired by PDE and ODE. The iteration procedure $H_{k+1} = (I + \eta L)^{-1} H_k \Theta_k$ is inspired by ODE theory on label propagation, as well as manifold learning motivated by PDE. The RBF and neural network based edge weights computation is also inspired by PDE and ODE.

Fig. 1. POGNN

Where $\Theta, \alpha$ is the parameter learned by the neural network.

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Calculate $w_{ij}$ using RBF

$$
e_{ij} = -\frac{||z_i - z_j||^2}{2\sigma^2}
= -\frac{2(1 - \cos(z_i, z_j))}{2\sigma^2}
de -\beta(1 - \cos(z_i, z_j)),
(49)
$$

$$
w_{ij} = \frac{\exp e_{ij}}{\sum_{k \in N(i)} \exp e_{ik}}
$$

where $\beta \in (0, 1)$ is a learnable parameter.

The proposed PDE and ODE inspired graph neural networks is shown on Fig. 1. It is so called POGNN. The iteration procedure $H_{k+1} = (I + \eta L)^{-1} H_k \Theta_k$ is inspired by ODE theory on label propagation, as well as manifold learning motivated by PDE. The RBF and neural network based edge weights computation is also inspired by PDE and ODE.

III. Subspace learning guided graph neural networks

A. Low-rank sparsity and manifold

1) Label propagation for subspace learning and semi-supervised learning on manifold: When there are few labeled samples, some assumptions must be made that relate the data distribution information revealed by the unlabeled samples to the class labels. The essence of the assumption is that "similar samples have similar outputs".

Definition 4 (Manifold assumption). Assuming that the data is distributed on a manifold, points on the same structure are more likely to have the same label value.

Definition 5 (Smoothness assumption). Assuming that two closely samples in a dense region have similar labels, otherwise, when they are separated by sparse data regions, their labels tend to be different.

Definition 6 (Cluster assumption). Assuming that the data has a cluster structure, samples in the same cluster belong to the same category, that is, points with similar distances have the same label.

The first and second assumptions consider the local consistency of points, and the third assumption considers the global consistency of points. These three assumptions stand for semi-supervised learning, and suggest that the data is distributed on subspace spanned through features.

Semi-supervised learning can be divided into two categories:

- Transductive learning: There is an intersection between unlabeled data and test samples, and the features of unlabeled data can be used for model training. The purpose of training is to give the optimal label to the unlabeled data in the current dataset.
- Inductive learning: There is no intersection between unlabeled data and test samples, the features of unlabeled data are not used for model training, and the purpose of training makes it applicable. The learner on unlabeled data has the best generalization performance.

Liu et al. proposed \cite{19} that sparse representation does not consider the global constraints of data, while low rank can reflect the global relationship of data, and when hidden data is added, low rank represents data that can still be effectively learned features.

$$
\min Z
\text{s.t. } X = AZ
(52)
$$
The problem is NP-hard, so a convex relaxation is performed and a noise term $E$ is added to give
\[
\min_{Z,E} \|Z\|_* + \lambda \|E\|_{2,1} \quad \text{s.t. } X = XZ + E
\] (53)

Where $\| \cdot \|_*$ represents the nuclear norm, that is, the sum of the singular values of the matrix. $\|E\|_{2,1} = \sum_j \sqrt{\sum_i e_{ij}^2}$ represents the $\ell_{2,1}$ norm, $\lambda > 0$.

High-dimensional features can be characterized by low-rank subspaces. Clustering high-dimensional data can be regarded as dividing it into different subspaces (subspace segmentation). Learning low-rank representation $Z$ from high-dimensional data $X$, instead of directly constructing adjacency matrix $W$ by $X$ in NCUT [26] and spectral clustering [20], the final $W = ([Z^*] + [Z^{**}])/2$.

NCut, spectral clustering, and low-rank representation are methods for constructing the topology of graphs entirely through features, while DeepWalk [22] is a method for learning node features on graphs entirely through topology. GCN [14] is a learning method that combines topology and feature matrix.

3) Low-rank representation and label propagation: In order to better derive the weight $W$ required for label propagation through $Z$, [41] adds constraints to solve the following optimization problem
\[
\min_{Z,E} \|Z\|_* + \lambda \|E\|_{2,1} \quad \text{s.t. } X = XZ + E, Z^T e = e, Z_{ij} = 0, \forall i, j \in \Omega
\] (54)

Where $e$ is a vector of all 1s, $\Omega$ is a set of edges, when $x_i, x_j$ are marked and are not in the same class, this constraint can be expressed as a projection operator $P_{\Omega}$, such that $P_{\Omega}(Z) = 0$.

In this way, the optimization problem can be written as in ADMM, remember
\[
A(Z) = \begin{pmatrix} \text{vec}(XZ) \\ Z^T e \\ P_{\Omega}(Z) \end{pmatrix}, B(E) = \begin{pmatrix} \text{vec}(E) \\ 0 \\ 0 \end{pmatrix}, c = \begin{pmatrix} \text{vec}(X) \\ 1 \\ 0 \end{pmatrix}
\] (55)

The vec operator means that the columns of the matrix are connected end to end and spliced into a longer column vector, then
\[
\min_{Z,E} \|Z\|_* + \lambda \|E\|_{2,1} \quad \text{s.t. } A(Z) + B(E) = c
\] (56)

B. Numerical optimization methods for subspace learning

1) Augmented Lagrangian multiplier: In [19], the augmented Lagrange multiplier method is used to solve the low-rank representation. And [18] is an improved Alternating Direction Method of Multipliers [2], that is, Linear Alternating Direction Method with Adaptive Penalty (LADMAP), to find low rank representation Methods.

[19] transforms the optimization problem (53) into
\[
\min_{Z,E} \|J\|_* + \lambda \|E\|_{2,1} \quad \text{s.t. } X = XZ + E, Z = J
\] (57)

The above optimization problem is solved using the augmented Lagrangian multiplier (ALM) method. The augmented Lagrangian function adds an F-norm term to the original Lagrangian function.
\[
\min_{Z,E,J,Y_1,Y_2} \|J\|_* + \lambda \|E\|_{2,1} + \text{tr}[Y_1^T(X - XZ - E)] + \text{tr}[Y_2^T(Z - J)] + \frac{\tau}{2}(\|X - XZ - E\|_F^2 + \|Z - J\|_F^2)
\] (58)

Theorem 9 (Singula Value Threshold). Optimization [5]
\[
\min_X \lambda \|X\|_* + \frac{1}{2} \|X - A\|_F^2
\] (59)

The solution is the SVT operator
\[
S_\lambda(A) = U \text{diag}(\max(0, s_i - \lambda)) V^T
\] (60)

where $USV^T$ is the singular value decomposition of $A$.

Theorem 10. Optimization [19]
\[
\min_W \lambda \|W\|_{2,1} + \frac{1}{2} \|W - Q\|_F^2
\] (61)

For the $i$ column, it corresponds to the following proximal operator optimization problem
\[
\min_{w_i} \lambda \|w_i\|_1 + \frac{1}{2} \|w_i - q_i\|_2^2
\] (62)

It is solved as
\[
S_\lambda(w_i) = \begin{cases} \frac{q_i}{\|q_i\|} q_i & \lambda < \|q_i\| \\ 0 & \text{otherwise} \end{cases}
\] (63)

The $S_\lambda$ in the above theorem is often called the shrinkage operator or the soft thresholding function.

2) Accelerated proximal gradient method: [18] gives the solution using accelerated proximal gradient (APG) [29] and proximal alternating direction method (i.e. ADMM with proximal operator) (53) process.

Consider the optimization problem $\min_X F(X) = P(X) + f(X)$. Do Taylor expansion of $F(X)$ at $Y$
\[
Q_\tau(X, Y) := f(Y) + \langle \nabla f(Y), X - Y \rangle + \frac{\tau}{2} \|X - Y\|_F^2 + P(X)
\]
\[
= \frac{\tau}{2} \|X - G\|_F^2 + P(X) + f(Y) - \frac{1}{2\tau} \|\nabla f(Y)\|_F^2
\] (64)

in
\[
G = Y - \tau^{-1} \nabla f(Y)
\] (65)

but
\[
\min_X F(X) = \min_X P(X) + \frac{\tau}{2} \|X - G\|_F^2
\] (66)

Here $P$ can be the nuclear norm, $\ell_{2,1}$ norm, etc. When $f(X) = \|AX - B\|_F^2/2, \nabla f(X) = AX - B$. The method of converting $\min_X F(X) = P(X) + f(X)$ into an optimization problem of the form (66) is called the proximal gradient method.

We use the speedup Nesterov trick, which is to set
\[
Y_k = X_k + \frac{t_k - 1}{t_k}(X_k - X_{k-1})
\] (67)
Theorem 11. In the above algorithm, when \( t_k = 1, \forall k \), the algorithm degenerates into the ordinary proximal gradient method, after iterating \( k \) times

\[
\exists L_f > 0, F(X_k) - F(X^*) \leq \frac{L_f \|X_0 - X^*\|^2}{2k}, \tag{68}
\]

That is to say, its convergence rate is \( O(1/k) \), where the Lipschitz constant \( L_f = \tau_k \). In other words, after \( O(L_f/\varepsilon) \) iterations, \( |F(X_k) - F(X^*)| \) converges to the order of \( \varepsilon \), so sometimes the convergence rate is also recorded as \( O(1/\varepsilon) \).

Theorem 12. In the above algorithm, when \( t_k \geq (k + 2)/2 \), the algorithm convergence rate is \( O(1/\sqrt{k}) \), that is, the convergence rate after iteration \( k \) is \( O(1/k^2) \).

Theorem 13. In the above algorithm, when \( t_{k+1}^2 - t_k^2 \leq t_k^2 \), the algorithm convergence rate is \( O(1/\sqrt{k}) \), the above formula takes the equal sign gets \( t_{k+1} = (1 + \sqrt{4t_k^2 + 1})/2 \).

3) Alternating Direction Method of Multipliers (ADMM) \[4\] Solve as

\[
\min_{x,z} f(x) + g(z) \tag{69}
\]

s.t. \( Ax + Bz = c \)

The optimization problem of augmented Lagrange multipliers

\[
L_\rho(x,z,y) = f(x) + g(z) + y^T(h(x,z)) + (\rho/2)\|h(x,z)\|^2_z \tag{70}
\]

\[
h(x,z) = Ax + Bz - c \tag{71}
\]

The iterative steps are

\[
x^{k+1} := \arg \min_x L_\rho(x,z^k,y^k) \tag{72}
\]

\[
z^{k+1} := \arg \min_z L_\rho(x^{k+1},z,y^k) \tag{73}
\]

\[
y^{k+1} := y^k + \rho(Ax^{k+1} + Bz^{k+1} - c) \tag{74}
\]

Remember the residual \( r = Ax + Bz - c \), then

\[
y^T r + (\rho/2)\|r\|^2_z = (\rho/2)\|r + (1/\rho)y\|^2_z - (1/2\rho)\|y\|^2_z \tag{75}
\]

\[
= (\rho/2)\|r + u\|^2_z - (\rho/2)\|u\|^2_z \tag{76}
\]

So there is the scaled form of ADMM

\[
x^{k+1} := \arg \min_x (f(x) + (\rho/2)\|Ax + Bz^k - c + u^k\|^2_z) \tag{77}
\]

\[
z^{k+1} := \arg \min_z (g(z) + (\rho/2)\|Ax^{k+1} + Bz - c + u^k\|^2_z) \tag{78}
\]

\[
u^{k+1} := u^k + Ax^{k+1} + Bz^{k+1} - c \tag{79}
\]

where \( u = y/\rho \).

Theorem 14 (ADMM convergence rate). ADMM converges under certain conditions (generally satisfied), its convergence rate is similar to that of ALM, which is \( O(1/k) \).

In practical operation, the convergence rate of ADMM is significantly slower than that of gradient descent, Newton’s method, etc. The main application of ADMM is when the size of the solution space is very large, such as a matrix of GB in storage space. At this time, many traditional methods are not easy to use, and it is forced to solve in blocks, and the absolute accuracy of the solution is often not so high. Also note:

1) ADMM generalized from 2-block to multi-block is not necessarily convergent.

2) In ADMM, when the value of \( \rho \) decreases with iteration, such as \[18\], it often works better, but it is also more difficult to analyze.

C. Ridge regression and LASSO

Definition 7 (Tikhonov regularization, \( \ell_2 \) regularization). Linear Least Squares Problem with Regularization of \( \ell_2 \) Norm

\[
\min_x \|Ax - b\|^2 + \lambda \|x\|^2 \tag{75}
\]

closed-form solution

\[
x^* = (A^T A + \lambda I)^{-1} A^T b \tag{76}
\]

Compared with the \( \ell_2 \) regularization, the \( \ell_1 \) regularization is less sensitive to outliers, and the obtained solution is more sparse. For example, in robust PCA \[9\], it is the optimization

\[
\min_{L,S} \|L\|_1 + \rho \|S\|_1 \tag{77}
\]

s.t. \( M = L + S \)

\( \ell_2 \) regularization and \( \ell_1 \) regularization are often referred to as ridge regression and LASSO (Least Absolute Shrinkage and Selection Operator), respectively.

The solution of LASSO can be obtained by the proximal gradient method, which is called iterative shrinkage thresholding algorithm (ISTA) \[8\].

Theorem 15 (ISTA). Linear Least Squares Problem with Regularization of \( \ell_1 \) Norm

\[
\min_x \|Ax - b\|^2 + \lambda \|x\|_1 \tag{78}
\]

solution

\[
x_{k+1} = S_{\lambda/\ell}(x_k - \frac{1}{\ell} A^T (Ax_k - b)) \tag{79}
\]

in

\[
S_{\lambda}(x) = \begin{cases} 
0 & |x| \leq \lambda \\
|x - \lambda \cdot \text{sign}(x)| & |x| > \lambda 
\end{cases} \tag{80}
\]

Theorem 16 (FISTA). The accelerated proximal gradient method is used in ISTA to obtain FISTA (fast iterative shrinkage thresholding algorithm) \[11\], and the convergence speed is increased from \( O(1/\varepsilon) \) to \( O(1/\sqrt{\varepsilon}) \).

D. Conditional random field for subspace graph neural networks

1) Conditional random field in machine learning on graph: Consider each node \( v_i \) on the graph as a factor \( x_i \) in the factor graph, remember \( x = (x_1, ..., x_n)^T \), compatibility function

\[
\psi(x) = \exp(-E(x)) \tag{81}
\]

Energy function

\[
E(x) = \frac{1}{2} (x - \mu)^T Q (x - \mu) \tag{82}
\]

Joint probability

\[
p(x) = \psi(x)/Z \tag{83}
\]
where normalized factor $Z = (2\pi)^{n/2}|Q|^{-1/2}$. Matrix $Q \in \mathbb{R}^{n \times n}$ is precision matrix, i.e. the inverse of covariance matrix. The normalized Laplacian matrix $L$ of a graph can be set as a precision matrix.

[31], [32] solves the weights of edges $w_{ij}$ through quadratic programming problem in local linear embedding (LLE).

$$\min \varepsilon = \sum_i \left\| x_i - \sum_{j:x_j \in N(x_i)} w_{ij}x_j \right\|^2$$

s.t. $\sum_{j:x_j \in N(x_i)} w_{ij} = 1, w_{ij} \geq 0$ (84)

In directed graph $w_{ij} \neq w_{ji}$.

$$\varepsilon = \left\| x_i - \sum_{j:x_j \in N(x_i)} w_{ij}x_j \right\|^2$$

$$= \left\| \sum_{j:x_j \in N(x_i)} w_{ij}(x_i - x_j) \right\|^2$$

$$= \sum_{j,k:x_j,x_k \in N(x_i)} w_{ij}w_{ik}(x_i - x_j)^T(x_i - x_k)$$

$$= \sum_{j,k:x_j,x_k \in N(x_i)} w_{ij}G_{jk}w_{ik}$$

where $G_{jk} = (x_i - x_j)^T(x_i - x_k)$ denotes Gram matrix of $x_i$. When Gram matrix is nearly singular, it can be estimated iteratively.

$$G^{(t+1)} = G^{(t)} + \varepsilon \cdot \text{trace}(G) \cdot I, 0 < \varepsilon \ll 1$$ (86)

Neighborhood $N(x_i)$ is defined through k-nearest principle. In state estimation or time-series forecasting problem, neighborhood denotes the points in time window, i.e. k-nearest neighborhood when time window width is k.

**Theorem 17.** The weights can be solved through

$$w_{ij} = \frac{\sum_{k \in N(i)} G_{jk}^{-1}}{\sum_{l \in N(i)} G_{ls}^{-1}}$$ (87)

The analytical solution given above requires the inversion of the Gram matrix, so this calculation method is not robust and requires a large amount of computation. In practical applications, numerical methods are often used to solve quadratic programming problems, such as active set method or interior point methods. To solve, or use a solver such as cvxopt. Appendix of proof of Theorem 17 provides a remark w.r.t. an iterative algorithm based on non-negative matrix factorization for solving this quadratic programming problem.

**Theorem 18.** For the conditional random field, when the increments are first-order, the energy function is the quadratic form of harmonic operator (normalized Laplacian matrix).

$$E = \frac{1}{2}x^TLx = \frac{1}{2} \sum_{i,j} w_{ij}(x_i - x_j)^2$$ (88)

**Theorem 19.** For the conditional random field, when the increments are second-order, the energy function is the quadratic form of biharmonic operator.

$$E = \frac{1}{2}x^TL^2x = -\frac{1}{2} \sum_{j \in N_i} (\sum_{j \in N_i} w_{ij}(x_j - x_i)^2)$$ (89)

**Theorem 20.** The expectation for conditional random field to estimate state $x$ from observation $y$ is

$$E[x|y] = -Q^{-1}xQ_{xy}y$$ (90)

2) Proposing GNN in CRF: For observations $y$ and states of latent variables $x$ in conditional random field (CRF), and according to Markov property in CRF, the state of a node is only related to its neighborhood. Hence, inference and inductive learning procedure on conditional random field as a graph, aggregate messages from neighborhood, which is intrinsically related to graph neural networks.

Currently, there has been a series of works combining variational inference with machine learning on graphs [23], [32]. Because variational inference needs to be modeled by conditional random fields (CRFs), it is natural to treat CRFs as graphs.

Consider the process of sampling $q(z)$ from $p(z, x)$. Assuming that the hidden variable on the node $k$ on the graph is $z_k$, by the mean field theory

$$q(z) = \prod_k q(z_k)$$ (91)

by the chain rule of conditional probability

$$p(z, x) = p(x) \prod_k p(z_k | z_{n \setminus k}, x)$$ (92)

Where $n \setminus k$ represents the set of all nodes on the graph except node $k$, so optimizing ELBO is equivalent to optimizing

$$L = \log p(x) + \sum_k q(z_k) \mathbb{E}_{q(z_{n \setminus k})}[\log p(z_k | z_{n \setminus k}, x)]$$

$$- \sum_k \mathbb{E}_{q(z_k)}[\log q(z_k)]$$ (93)

Derivation of the functional $L$ using the variational method

$$\frac{\partial L}{\partial q(z_k)} = \mathbb{E}_{q(z_{n \setminus k})}[\log p(z_k | z_{n \setminus k}, x)] - \log q(z_k) - 1 = 0$$ (94)

have to

$$\log q(z_k) = \mathbb{E}_{q(z_{n \setminus k})}[\log p(z_k | z_{n \setminus k}, x)] + \text{const}$$ (95)

This means that

$$q(z_k) \propto \exp \left( \mathbb{E}_{q(z_{n \setminus k})}[\log p(z_k | z_{n \setminus k}, x)] \right)$$ (96)

This means that we need to sample from all nodes in the graph except node $k$ to find $q(z_k)$. This will be very troublesome when the number of nodes in the whole graph is large.

**Theorem 21.** The process of obtaining $q(z_k)$ by sampling from all nodes on the graph except node $k$, you can obtain $q(z_k)$ by sampling from the neighborhood $N(k)$ of node $k$ to replace [23], [32], that is

$$q(z_k) \propto \exp \left( \mathbb{E}_{q(z_{N(k)})}[\log p(z_k | z_{N(k)}, x)] \right)$$ (97)

According to the mean field assumption, that is, the hidden variables are independent of each other, and there are

$$q(z_k) \propto \exp \left( \mathbb{E}_{q(z_{N(k)})}[\log p(z_k, z_{N(k)}, x)] \right)$$ (98)
In other words, it is also possible to sample from the joint distribution of node $k$ and its neighbors $N(k)$.

The formula of the $l$-th ($l > 0$) graph convolutional layer is

$$H^{(l)} = \rho(\tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2} H^{(l-1)} \Theta^{(l)})$$

(99)

where $\tilde{A}$ is adjacency matrix with self-loop, i.e. $\tilde{A} = A + I$. $\tilde{D}$ is a diagonal matrix called degree matrix, $D_{ii} = \sum_j \tilde{A}_{ij}$, $\rho(\cdot)$ denotes nonlinear activation function, $\Theta^{(l)}$ denotes weight of the $l$-th layer of network, and $H^{(0)}$ is the initial input feature matrix. Let $\tilde{A} = D^{-1/2} \tilde{A} D^{-1/2}$, then

$$H^{(l)} = \rho(\tilde{A} H^{(l-1)} \Theta^{(l)})$$

(100)

denotes first-order aggregation, while

$$H^{(l)} = \rho(\tilde{A}^2 H^{(l-1)} \Theta^{(l)})$$

(101)

denotes second-order aggregation. For CRF-GNN, the message passing procedure of GNN is illustrated as the following formula:

$$h^{(k)}_i = \frac{1}{d_i + 1} h^{(k-1)}_i + \sum_{j=1}^{n} \frac{1}{(d_i + 1)(d_j + 1)} h^{(k-1)}_j$$

(102)

3) Inductive learning: The CRF algorithm on graph is easy to implement inductive learning. For a new point $x_o$

$$E[x_o|x] = -q_o^{-1} q_{on} y$$

(103)

where $q_{on} = (q_{o1}, q_{o2}, \ldots)$.

If states are biased,

$$x - b_x \sim N(0, 1/\lambda)$$

(104)

where $0 < \lambda < 1$, then suppose

$$\tilde{x}_i \sim N(0, 1/(1-\lambda))$$

(105)

For joint distribution $p(y, x, b_x)$

$$Q = (1 - \lambda) \begin{pmatrix} Q_{yy} & Q_{yx} & 0 \\ Q_{xy} & Q_{xx} & 0 \\ 0 & 0 & 0 \end{pmatrix} + \lambda \begin{pmatrix} 0 & 0 & 0 \\ 0 & I & -I \\ 0 & -I & I \end{pmatrix}$$

(106)

i.e.

$$Q = \begin{pmatrix} (1 - \lambda)Q_{yy} & (1 - \lambda)Q_{yx} & 0 \\ (1 - \lambda)Q_{xy} & (1 - \lambda)Q_{xx} + \lambda I & -\lambda I \\ 0 & -\lambda I & \lambda I \end{pmatrix}$$

(107)

Then, calculate $E(x|y, b_x)$ is equivalent to solve linear equation

$$\begin{pmatrix} (1 - \lambda)Q_{yy} & (1 - \lambda)Q_{yx} & 0 \\ (1 - \lambda)Q_{xy} & (1 - \lambda)Q_{xx} + \lambda I & -\lambda I \\ 0 & -\lambda I & \lambda I \end{pmatrix} \begin{pmatrix} y \\ x \\ b_x \end{pmatrix} = 0$$

(108)

This problem can be relaxed into linear least square problem. If observations are biased,

$$y - b_y \sim N(0, \lambda)$$

(109)

By $\tilde{x}_i \sim N(0, 1/(1-\lambda))$, for $p(y, x, b_y)$

$$Q = (1 - \lambda) \begin{pmatrix} Q_{yy} & Q_{yx} & 0 \\ Q_{xy} & Q_{xx} & 0 \\ 0 & 0 & 0 \end{pmatrix} + \lambda \begin{pmatrix} I & 0 & I \\ 0 & 0 & 0 \\ -I & 0 & I \end{pmatrix}$$

(110)

i.e.

$$Q = \begin{pmatrix} (1 - \lambda)Q_{yy} + \lambda I & (1 - \lambda)Q_{yx} & -\lambda I \\ (1 - \lambda)Q_{xy} & (1 - \lambda)Q_{xx} & 0 \\ 0 & 0 & \lambda I \end{pmatrix}$$

(111)

Then calculate $E(x, y|b_y)$ is equivalent to

$$\begin{pmatrix} (1 - \lambda)Q_{yy} + \lambda I & (1 - \lambda)Q_{yx} & -\lambda I \\ (1 - \lambda)Q_{xy} & (1 - \lambda)Q_{xx} & 0 \\ 0 & 0 & \lambda I \end{pmatrix} \begin{pmatrix} y \\ x \\ b_y \end{pmatrix} = 0$$

(112)

E. Classifier based on VGAE-guided subspace graph neural networks

1) Learning from label propagation to GNN: Both label propagation algorithms and graph neural networks can be widely used in weakly supervised problems. The convergence of the label propagation algorithm is derived from the Perron-Frobenius theorem, and [24] proves the convergence of graph neural networks, which can be guaranteed by Banach’s fixed point theorem.

The label propagation algorithm can only detect the subspace well when the node feature dimension is low, while the graph neural network is better at capturing information from high-dimensional, sparse features. It can be explored to use the graph neural network to first roughly estimate the subspace for dimensionality reduction before label propagation.

2) Variational graph autoencoder and subspace learning: Variational graph autoencoder (VGAE) [15] is a method of adding GCN to the encoding-decoding structure and variational inference to learn the low-dimensional and low-rank representation of node features on the graph [27]. We can first use the high-dimensional feature $X$ to roughly estimate an adjacency matrix $W_0$, then input $W_0$ and $X$ into VGAE, learn the low-dimensional representation $\mu$, and calculate it by $\mu$ New $W$ for the label propagation process. Based this idea, this paper designs three tentative networks that combine GCN and label propagation via subspace learning for node classification on Cora. The procedure is on Appendix.

IV. Conclusions

Probabilistic theory and differential equations are essential for understanding and guiding the design of machine learning models, particularly for understanding the mathematical basis of learning latent variables from observations. Subspace learning maps high-dimensional features onto low-dimensional subspaces to create an efficient representation. Graphs are often used to model latent variable learning problems, and graph neural networks implement deep learning architectures on graphs. This paper draws on probabilistic theory and differential equations to provide insights and suggestions on how graph neural networks can be used to solve subspace learning problems through variational inference and differential equations.
APPENDIX A
SUMMARY OF SUBSPACE LEARNING ALGORITHMS

1) Low Rank Representation
   - Measurement $\min_Z \text{rank}(Z)$ s.t. $X = XZ$
   - Convex Surrogate $\min_{Z,E} \|Z\|_*$ + $\lambda \|E\|_1$ s.t. $X = XZ + E$
   - Methods ALM, APG, ADMM, LADMAP

2) Matrix Completion
   - Measurement $\min_M \text{rank}(M)$ s.t. $P_M(M) = P_M(A)$
   - Convex Surrogate $\min_M \|M\|_*$ s.t. $P_M(M) = P_M(A)$
   - Methods APG

3) Principal Component Analysis (PCA)
   - Measurement $\max_W \text{trace}(W^TXX^TW)$ s.t. $W^TW = I$
     - i.e. $\min_{W,H} \|X-WH\|_F^2$ s.t. $W^TW = I$
     - Minimum projection distance of the samples
     - Maximum projection variance of the samples
     - PCA is a low rank model $\min_L \text{rank}(L) \leq k \|X-L\|_F^2$, thus it equals singular value thresholding in its result.
   - Methods Eigenvalue Decomposition

4) Linear Discriminant Analysis (LDA)
   - Measurement $\max_W \text{trace}(W^TS_wW)/\text{trace}(W^TS_bW)$
   - Methods Generalized Eigenvalue Decomposition

5) Robust PCA
   - Measurement $\min_{L,S} \|L\|_* + \rho \|S\|_1$ s.t. $M = L + S$
   - Methods ADMM, here it calls robust principal component pursuit (RPCP)

6) Sparse Subspace Clustering
   - Measurement $\min_Z \|Z\|_0$ s.t. $X = XZ$
   - Convex Surrogate $\min_Z \|Z\|_1$ s.t. $X = XZ$
   - Methods ALM, APG

7) Sparse Coding
   - Measurement $\min_{D,X} \|Y-DX\|_F^2 + \lambda \|X\|_1$, usually calls LASSO (Least Absolute Shrinkage and Selection Operator).
   - Methods ADMM
     - Update $X$, called sparse coding, and methods include match pursuit (a kind of greedy algorithm), ISTA, FISTA etc.
     - Update $D$, called dictionary learning, usually use Method of Optimal Directions (MOD) or K-SVD

8) Normalized Cuts / Laplacian Eigenmaps / Spectral Clustering
   - Measurement $\min_{y \mathcal{L}Y}$, where $\mathcal{L}$ denotes normalized Laplacian Matrix.
   - Methods Eigenvalue Decomposition, the second smallest eigenvector of $L$ is the real valued solution, since the smallest eigenvalue of $L$ is 0 with an all-one eigenvector.

9) Non-negative matrix factorization (NMF)

- Measurement $\min_{W \geq 0, H \geq 0} D[X][WH]$, where $D[A||B]$ denotes the divergence between $A$ and $B$
  - Frobenius divergence, $D[X||WH] = \|X - WH\|_F^2$, is a maximum likelihood estimator due to the additive Gaussian noise, usually used.
  - KL divergence, $D[X||WH] = \sum_{i,j} X_{ij} \ln(\frac{X_{ij}}{WH_{ij}}) - X_{ij} + (WH)_{ij}$, is maximum likelihood for the Poisson process.
  - Graph NMF, $\min_U \|X - UV^T\|_F^2$ + $\text{trace}(VLV^T)$
  - Methods Multiply Iteration

10) Local Linear Embedding (LLE)
    - Measurement $\min \text{trace}(ZQZ^T)$ s.t. $ZZ^T = I$, where $Q = (I-W)^T(I-W)$, and here the normalized Laplacian is $L = I - W$
    - Methods Eigenvalue Decomposition

11) Support Vector Machine (SVM)
    - Measurement Maximize the margin
      - Kernel SVM, the primal problem is $\min_{w,b} \frac{1}{2} \|w\|^2$ s.t. $y_i(w^Tf(x_i) + b) \geq 1$. The dual problem is $\max_{\alpha} \sum_{i} \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j k(x_i, x_j)$ s.t. $\sum_i \alpha_i y_i = 0$, $\alpha_i \geq 0$, where kernel function $k(x_i, x_j) = f^T(x_i) f(x_j)$.
      - Soft margin SVM, $\max_{\alpha} \sum_{i} \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j k(x_i, x_j)$ s.t. $\sum_i \alpha_i y_i = 0$, $C \geq \alpha_i \geq 0$, equivalent to $\min_{\alpha, \xi} \frac{1}{2} \|\alpha\|^2 + C \sum_i \xi_i + \gamma \alpha^T K \alpha$ s.t. $y_i(\sum_j \alpha_j k(x_i, x_j) + b) \geq 1 - \xi_i$, $\xi_i \geq 0$
      - Transductive SVM is applied to solve semi-supervised learning problem. The key idea is to assign a pseudo-label to each unlabeled data first, then iteratively correct the labels.
      - Laplacian SVM, suppose $u$ and $l$ denote number of unlabeled and labeled data, optimize $\min_{\alpha, \xi} \frac{1}{2} \|\alpha\|^2 + \gamma \alpha^T K \alpha + \lambda \|\alpha\|_1$ s.t. $\sum_j \alpha_j k(x_i, x_j) + b \geq 1 - \xi_i$, $\xi_i \geq 0$
    - Methods Sequential Minimum Optimization (SMO)

12) Multiple Dimensional Scaling (MDS) / IsoMAP (Isometric Feature Mapping)
    - Measurement $\min_Y \|G - Y^TY\|_F^2$, where $G_{ij} = \langle x_i, x_j \rangle$ is the Gram matrix, that can be computed from pairwise distances.
      - PCA and MDS are in some sense dual to each other. Suppose $X \in \mathbb{R}^{D \times N}$, in PCA, we compute the $D \times D$ covariance matrix $XX^T$. In MDS, we compute the $N \times N$ Gram matrix. For Euclidean distances, the two methods yield the same embedding results (up to an arbitrary rotation).
      - In IsoMAP we use geodesic distances rather than Euclidean distances in MDS. After constructing a graph, we apply Dijkstra all-pairs shortest-paths algorithm to compute the distances.
    - Methods Eigenvalue Decomposition of Gram matrix, $G = VAV^T$, then $Y^* = \Lambda^{1/2}V^T$. 
13) Label Propagation (LP)

- **Measurement** \( \min_{F} F^T L F + \gamma \| F - Y \|_F^2 \), considering normalized Laplacian is \( L = I - W \), the optimal solution is \( F^* = (1 - \alpha)(I - \alpha W)^{-1} Y \), where \( \alpha = 1/(1 + \gamma) \).

- **Methods** Iteration \( F^{(k)} = \alpha W F^{(k-1)} + (1 - \alpha) Y, 0 < (1 - \alpha) \ll 1 \).

14) Regularized Least Square (RLS)

- **Measurement** Minimize Mean Square Errors

  - Tikhonov Regularization, \( \min_{x} \|Ax - b\|_2^2 + \lambda \|Lx\|_2^2 \Rightarrow x^* = (AT_A + L^T L)^{-1} A^T b \), also calls ridge regression.

  - Laplacian RLS, \( \min_{x} F^T F + \gamma \| F - Y \|_F^2 + \lambda \| F \|_F^2 \), the optimal solution is \( F^* = (1 - \alpha)(I - \alpha W)^{-1} Y \), where \( \alpha = 1/(1 + \gamma + \lambda) \).

15) Probabilistic Matrix Factorization (PMF)

- **Measurement** \( \min_{U,V} \| R - U^T V \|_F^2 \) s.t. \( P_{13}(R) = P_{13}(U^T V) \), where \( R \sim N(U^T V, \sigma^2 I), U \sim N(0, \sigma_u^2 I), \) \( V \sim N(0, \sigma_v^2 I) \), \( \min_{U,V} \lambda_p \| R - U^T V \|_F^2 + \frac{\lambda_p}{\|U\|_2^2 + \lambda_p}\|V\|_2^2 \), it is regularized SVD where \( \lambda_U = \sigma^2/\sigma_u^2, \lambda_V = \sigma^2/\sigma_v^2 \).

**APPENDIX B**

**PROOF OF THEOREMS**

**Proof of Theorem 1**

Proof. \( \Delta(y) = \nabla \cdot \nabla y = \text{div} \nabla y, \int_M < X, \nabla y > = \int_M \text{div}(X)y \) (113)

So \( \int_M \|\nabla y\|^2 = \int_M \Delta(y)y \) (114)

So \( \min y^T \Delta y \Leftarrow \min \|\nabla y\|^2 \) (115)

**Proof of Theorem 2**

Proof. We regard the label information as the temperature on the graph. When the “thermal equilibrium” is reached, that is, when the label propagation converges, there will be \( \Delta u = 0 \). Let \( u(x,0) = f(x) \) be the initial heat distribution, and solve the problem of partial differential equation \( 10 \) according to this initial condition, which is called the Cauchy problem of heat conduction equation. The special solution of \( 10 \) when \( f(x) = \delta(x) \) is

\[ \Phi_t(x) = \frac{1}{(4\pi t)^{n/2}} \exp \left( -\frac{\|x\|^2}{4t} \right), t > 0 \] (116)

This is also known as the fundamental solution of the heat conduction equation, and

\[ \int_{\mathbb{R}^n} \Phi_t(x)dx = 1 \] (117)

Let \( H_t(x,y) = \Phi_t(x-y) \), the solution of \( 10 \) is

\[ u(x,t) = \int_M H_t(x,y)f(y)dy \] (118)

That is, the convolution of the kernel \( H_t \) and the initial condition \( f(x) \). So

\[ \Delta f(x) = \frac{\partial}{\partial t} \left( \int_M H_t(x,y)f(y)dy \right) \bigg|_{t=0} \]

\[ = \frac{1}{t} (f(x) - g(x,y)) \] (119)

\[ g(x,y) = (4\pi t)^{-n/2} \int_M \exp \left( -\frac{\|x-y\|^2}{4t} \right) f(y)dy \] (120)

For a point \( x_i \), assuming that there are \( k \) points in its neighborhood, then

\[ \Delta f(x_i) = -\frac{1}{t} (f(x_i) - g(x_i, x_j)) \] (121)

\[ g(x_i, x_j) = \frac{1}{k} (4\pi t)^{-n/2} \sum_{j \in N(i)} \exp \left( -\frac{\|x_i-x_j\|^2}{4t} \right) f(x_j) \] (122)

where \( N(i) = \{x_j | 0 < \|x_i-x_j\| < \varepsilon \} \), when \( \Delta f(x_i) \approx 0 \)

\[ \frac{1}{k} (4\pi t)^{-n/2} \sum_{j \in N(i)} \exp \left( -\frac{\|x_i-x_j\|^2}{4t} \right) = 1 \] (123)

so

\[ w_{ij} = \exp \left( -\frac{\|x_i-x_j\|^2}{4t} \right) \] (124)

**Proof of Theorem 3**

Proof. Consider the iterative process of label propagation \( y^{(t)} = \alpha Wy^{(t-1)} + (1 - \alpha)y^{(0)}, \alpha \approx 1, \) then

\[ \begin{pmatrix} y_{u}^{(t)} \\ y_{l}^{(t)} \end{pmatrix} \approx \begin{pmatrix} W_{uu} & W_{ul} \\ W_{lu} & W_{ll} \end{pmatrix} \begin{pmatrix} y_{u}^{(t-1)} \\ y_{l}^{(t-1)} \end{pmatrix} \] (125)

\[ y_{u}^{(t)} \approx W_{uu}y_{u}^{(t-1)} + W_{ul}y_{l} \] (126)

The general solution to this difference equation is

\[ y_{u}^{(t)} = W_{uu}^{t}\bar{y}_{u}^{(0)} + \left( \sum_{i=1}^{t} W_{uu}^{i-1} \right) W_{ul}\bar{y}_{l} \] (127)

Because the spectral radius \( \rho(W_{uu}) < 1 \), so \( \lim_{t \to \infty} W_{uu}^{t} = 0 \) (this shows that the final estimation result of \( y_{u}^{(t)} \) has little effect, usually set \( y_{u}^{(0)} = 0 \), and because \( \lim_{t \to \infty} \sum_{i=1}^{t} W_{uu}^{i-1} = (I - W_{uu})^{-1} \), so

\[ y_{u}^{*} = (I - W_{uu})^{-1} W_{ul} \bar{y}_{l} \] (128)

And because \( Q = I - W \), so \( Q_{uu} = I - W_{uu}, Q_{ul} = -W_{ul} \), namely \( y_{u}^{*} = -Q_{uu}^{-1} Q_{ul} \bar{y}_{l} \).

**Proof of Theorem 6**

Proof. \( \rho(D^{-1}A) = 1 \), so the eigenvalue of \( D^{-1}A \) is located in the \([-1, 1]\) interval, obviously, for (the number of nodes For
any graph not less than 2), $D^{-1}A$ has an eigenvalue of 1, and the corresponding eigenvector is

$$(1, 1, \ldots, 1)^T$$

Only for the bipartite graph, $D^{-1}A$ has the eigenvalue $-1$, assuming that the two parts of the bipartite graph have $a, b$ nodes respectively, then the eigenvalue $-1$ corresponds to The eigenvector is

$$(1, 1, \ldots, 1, -1, -1, \ldots, -1)^T$$

And because

$$x^T L_{rw}x = 1 - x^T D^{-1} Ax$$

(129)

So we can get Theorem.

Proof. Notice that

$$
\rho(\tilde{D}^{-1/2} A \tilde{D}^{-1/2}) = \frac{d_m}{d_m + 1}
$$

so

$$
\min_{\|x\|=1} x^T \tilde{D}^{-1/2} A \tilde{D}^{-1/2} x \geq -\frac{d_m}{d_m + 1}
$$

From this, we can directly get

$$
\tilde{\lambda}_n \leq 1 - \frac{1}{d_m + 1} - \left(-\frac{d_m}{d_m + 1}\right) = \frac{2d_m}{d_m + 1}
$$

This approximation can significantly reduce the amount of computation for $\tilde{\lambda}_n$, in fact, $\tilde{d}$ is the quotient of the total number of edges divided by the total number of nodes, in other words, the sum of adjacency matrix elements divided by the matrix order’s business.

For undirected weighted graphs, because $\tilde{d}$ is large, $\beta_1$ is also large, so the above estimation formula does not apply.

For directed graphs, the above estimator does not apply.

Cora dataset [25], $n_t = 140, n = 2708$, when no self-loop is added, $\tilde{d} = 10858/2708 = 4.00, d_m = 168, d_{min} = 1, \beta_1 = -1$, the arithmetic mean of After adding the self-loop $\tilde{\lambda}_n = 1.4826$.

Citeseer dataset [25], $n_t = 120, n = 3327$, when no self-loop is added, $\tilde{d} = 2.7364, d_m = 99, d_{min} = 0$, after adding self-loop $nlde\tilde{\lambda}_n = 1.5022$. In the Citeseer dataset, when the self-loop is not added, the degree of dozens of points is 0, which affects the estimation result.

Pubmed dataset [25], $n_t = 60, n = 19717$, when no self-loop is added, $\tilde{d} = 4.4960, d_m = 171, d_{min} = 1$, the arithmetic mean of After adding the self-loop $\tilde{\lambda}_n = 1.650$.

Remark of Theorem 8 From the perspective of GCN, $Y$ is also a graph signal, and the filter corresponding to the label propagation algorithm is an auto-regressive filter $p_{ar}(\lambda) = 1/(1 + \alpha \lambda)$. The features of nodes on the graph can be regarded as a generalized label, which puts the label propagation algorithm and GCN under a unified framework.

Proof. GCN can be written as

$$H^{(t+1)} = \sigma(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(t)} W^{(t)})$$

(130)

where $\tilde{A} = A + I$. Matrix $\tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2} = I - \tilde{D}^{-1/2} \tilde{L} \tilde{D}^{-1/2}$ corresponds to the renormalization filter (renormalization filter, RNM) $p_{rnm}(\lambda) = (1 - \lambda)^k$. Two kinds of graph neural networks can be designed for this purpose, namely generalized label propagation. Note that the re-regularization technique is not used here, but is obtained directly from [77].

$$H^{(t+1)} = \sigma((I + \alpha D^{-1/2} LD^{-1/2})^{-1} H^{(t)} W^{(t)})$$

(131)

and, enhanced graph convolution networks

$$H^{(t+k)} = \sigma((I - \tilde{D}^{-1/2} \tilde{L} \tilde{D}^{-1/2})^k H^{(t)} W^{(t)})$$

(132)

It is equivalent to simplify graph convolution (SGC) [33].

Before inputting the feature $X$ into the graph neural network, first use AR or RNM filter to filter it to obtain the filtered feature $\tilde{X}$, and then set $H^{(0)} = \tilde{X}$.

$$\tilde{X}_{ar} = (I + \alpha D^{-1/2} LD^{-1/2})^{-1} \tilde{X}$$

(133)

$$\tilde{X}_{rnm} = (I - \tilde{D}^{-1/2} \tilde{L} \tilde{D}^{-1/2})^k \tilde{X}$$

(134)

When the matrix $L$ is large, in order to avoid the computational complexity caused by the direct inversion of $(I + \alpha D^{-1/2} LD^{-1/2})$ too high, by

$$(I + \alpha D^{-1/2} LD^{-1/2})^{-1} = \frac{1}{1 + \alpha} \sum_{i=0}^{+\infty} \left(\frac{\alpha}{1 + \alpha} D^{-1/2} AD^{-1/2}\right)^i$$

(135)

So take iterative

$$X^{(0)} = O, \ldots, X^{(i+1)} = X + \frac{\alpha}{1 + \alpha} D^{-1/2} AD^{-1/2} X^{(i)}$$

(136)

then make

$$\tilde{X}_{ar} = \frac{1}{1 + \alpha} X^{(i)}$$

(137)

When $t = [4\alpha]$, a better estimate can be obtained.

Proof of Theorem 13

Proof.

$$t_{k+1} = 1 + \frac{\sqrt{4t_k^2 + 1}}{2} > 1 + \frac{2t_k}{2} = t_k + \frac{1}{2}$$

(138)

Take $t_0 = 1$ then $t_k > 1 + k/2 = (2 + k)/2$.

Proof of Theorem 17

Proof. For node $i$

$$\min_{w_i} \frac{1}{2} w_i^T G^i w_i + \text{s.t. } e^T w_i = 1$$

(139)

Lagragian multiplier

$$L^i = \frac{1}{2} w_i^T G^i w_i - \lambda_i (e^T w_i - 1) = 0$$

(140)

Through KKT condition

$$\nabla_{w_i} L^i = G^i w_i - \lambda_i e = 0, \nabla_{\lambda_i} L^i = e^T w_i - 1 = 0$$

(141)
Note \( G^{-1} = (G^T)^{-1} \)
\[
    w_i = G^{-1} \begin{pmatrix} (\lambda_i) \\ \vdots \\ (\lambda_i) \end{pmatrix}, \quad w_{ij} = \lambda_i \sum_{k \in N(i)} G^{-1}_{jk} \tag{142}
\]
and \( \sum_j w_{ij} = 1 \), so
\[
    w_{ij} \leftarrow \frac{\lambda_i \sum_{k \in N(i)} G^{-1}_{jk}}{\sum_{j \in N(i)} (\lambda_i \sum_{k \in N(i)} G^{-1}_{jk})} = \frac{\sum_{k \in N(i)} G^{-1}_{jk}}{\sum_{LS \in N(i)} G^{-1}_{ls}} \tag{143}
\]

Remark of Theorem 17: There is an iterative algorithm based on non-negative matrix factorization for solving this quadratic programming problem [38].

Proof. Eq. (84) is equivalent to
\[
    \min_{\mathbb{W}} \frac{1}{2} \|X - (C \odot W)X\|_F^2 + \frac{\mu}{2} \sum_{i=1}^m \|(C \odot W)e_i - e\|_F^2 - \sum_{i \in N(i)} (C_{ij} \odot e_{ij}) \tag{144}
\]
where \( C_{ij} = \begin{cases} 1 & x_j \in N(x_i), \odot \text{ denotes Hadamard product} \\ 0 & \text{otherwise} \end{cases} \) and \( e = [1, 1, \ldots, 1]^T \). Lagrangian multiplier
\[
    L = \frac{1}{2} \|X - (C \odot W)X\|_F^2 + \frac{\mu}{2} \|(C \odot W)e\|_F^2 - L^P \tag{145}
\]
\[
    L^P = \lambda^T ((C \odot W)e - e) - \text{trace}(\Phi^T \mathbb{W}) \tag{146}
\]
So
\[
    \nabla_w L = (C \odot (C \odot W)X)X^T + \mu(C \odot W)e e^T - X^T X^T - \lambda^T e e^T - \Phi \tag{147}
\]
By KKT condition \( \phi_{ij} w_{ij} = 0, \nabla_w L = 0 \) so
\[
    C_{ij}((C \odot W)X X^T + \mu(C \odot W)e e^T - X^T X^T - \lambda^T e e^T)_{ij} W_{ij} = 0 \tag{148}
\]
Hence
\[
    W_{ij} = \begin{cases} W_{ij} & (XX^T + \lambda^T e e^T)_{ij} \\ 0 & \text{otherwise} \end{cases} \tag{149}
\]
or \( W_{ij} = 0 \) when \( x_j \notin N(x_i) \). For node \( i \),
\[
    \min_{w_i} \frac{1}{2} w_i^T G^i w_i + \frac{\mu}{2} \|w_i\|_1^2 \quad \text{s.t.} \quad e^T w_i = 1, w_i \geq 0 \tag{150}
\]
Lagrange multiplier
\[
    L' = \frac{1}{2} w_i^T G^i w_i + \frac{\mu}{2} \|w_i\|_1^2 - \lambda_i (e^T w_i - 1) - \eta^T w_i \tag{151}
\]
KKT condition
\[
    \nabla_{w_i} L' = G^i w_i + \mu e e^T w_i - \lambda_i e - \eta = 0 \tag{152}
\]
\[
    \nabla_{\lambda_i} L' = e^T w_i - 1 = 0 \tag{152}
\]
\[
    \eta \geq 0, w_i \geq 0, \eta w_{ix} = 0 \tag{152}
\]
so
\[
    w_i^T \nabla_{w_i} L' = w_i^T G^i w_i + \mu(w_i^T e)^2 - \lambda_i w_i^T e = 0 \tag{153}
\]
so
\[
    \lambda_i = (w_i^T G^i w_i + \mu(e^T w_i)^2)/e^T w_i \tag{154}
\]

Proof of Theorem 18

Proof. First-order increment
\[
    \dot{x}_i = x_i / \sqrt{\sum_i w_{ji} - x_j / \sqrt{\sum_j w_{ij} = x_i - x_j}} \tag{157}
\]
If \( e \) is an all-one vector, then \( Q \) satisfies \( Qe = 0 \), and because \( \sum_j w_{ij} = 1 \), it can be assumed that \( d_{ij} \sim N(0, 1/w_{ij}) \), where \( w_{ij} \) represents the edge weights, assuming that the increments are independent, the joint probability distribution of \( x \)
\[
    p(x) \propto \prod_{(i,j) \in E} p(\dot{x}_{ij}) \tag{158}
\]
\[
    \propto \prod_{(i,j) \in E} \exp(-\frac{1}{2} w_{ij}(x_i - x_j)^2) \tag{158}
\]
\[
    = \exp(-\frac{1}{2} \sum_{(i,j) \in E} w_{ij}(x_i - x_j)^2) \tag{158}
\]
\[
    = \exp(-\frac{1}{2} e^T L x) \tag{158}
\]

Proof of Theorem 19

Proof. For a graph with \( n \) nodes, we introduce \( n \) hyperedge nodes, and the hyperedge node \( e_i \) contains all nodes \( v_i \) and \( v_i \)’s neighborhood set \( N(i) \) node. The labels of the hypernodes are weighted and summed by the node labels in \( N(i) \), that is, \( \sum_{j \in N_i} w_{ij} \), so for the second order, the increment is defined as the difference between the hypernode and its corresponding node
\[
    \ddot{x}_i = x_i - \sum_{j \in N_i} w_{ij} x_j \tag{159}
\]
where \( \sum_{j \in N_i} w_{ij} = 1 \). For the precision matrix \( Q^h = \text{diag}\{\ddot{x}_i\} \) of the hypergraph, there is still \( Q^h e = 0 \), and \( e \) is an all-one vector, so it can be assumed that \( d_i \sim N(0, 1) \), then
\[
    p(y) \propto \prod_i p(\ddot{x}_i) \tag{160}
\]
\[
    \propto \exp(-\frac{1}{2} \sum_i (\sum_{j \in N_i} (w_{ij} - x_i)^2) \tag{160}
\]
\[
    = \exp(-\frac{1}{2} x^T (I - W)^T (I - W)x) \tag{160}
\]
\[
    = \exp(-\frac{1}{2} x^T L^T L^T x) \tag{160}
\]
Proof. Consider the joint distribution of state $x$ and observation $y$

$$Q^{-1} = \begin{bmatrix} Q_{xx} & Q_{xy} \\ Q_{yx} & Q_{yy} \end{bmatrix}^{-1} = \begin{bmatrix} C_1^{-1} & -Q_{yx}C_2^{-1} \\ -C_2^{-1}Q_{yx} & C_1^{-1} \end{bmatrix}$$

$$= \Sigma = \begin{bmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{bmatrix}$$

(161)

$\Sigma$ denotes covariance matrix.

$$C_1 = Q_{xx} - Q_{xy}Q_{yy}^{-1}Q_{yx}$$

$$C_2 = Q_{yy} - Q_{yx}Q_{xx}^{-1}Q_{xy}$$

(162)

When

$$\begin{pmatrix} x \\ y \end{pmatrix} \sim N \left( \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \begin{bmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{bmatrix} \right)$$

(163)

and

$$p(x|y) = N(\mu_x + \Sigma_{xy}^{-1}(y - \mu_y), \Sigma_{xx} - \Sigma_{xy}\Sigma_{yy}^{-1}\Sigma_{yx})$$

(164)

and $\mu_x = \mu_y = 0$, so

$$E[x|y] = -Q_{xx}^{-1}Q_{xy}y$$

(165)

**APPENDIX C**

**SUPPLEMENTARY MATERIALS**

Cora dataset [25] has a total of 2708 sample points, each sample point is a paper, and all sample points are divided into 7 categories. Each paper is represented by a 1433-dimension word vector to represent its feature vector. Each element of the word vector corresponds to a word, and the element has only two values of 0 or 1. Take 0 to indicate that the word corresponding to this element is not in the paper, and take 1 to indicate that it is in the paper. The citation relationship of the paper is the edge of the graph, and there are no isolated points on the graph. Only a small number of sample points (140 points) in the dataset are labeled with class labels, so the classification problem belongs to semi-supervised classification.

A. **Label propagation parameter selection in POGNN**

Conduct the following experiments on the Cora dataset, setting $\text{dim}=16$, learning rate=0.1, weight decay = 5e-4, epoch=50. The propagation process $H_{k+1} = A H_k \Theta_k$, Accuracy:

- $A = I - \eta L$, where
  - $\eta = 0.5$: 0.757
  - $\eta = 0.66$: 0.784
  - $\eta = 1$: 0.812
  - $\eta = 1.5$: 0.826
  - $\eta = 2$: 0.837
  - $\eta = 5$: 0.834

Convert the solution equation $L f = 0$ into the solution differential equation $df/dt = -L f$, $f_0 = y$ (similar to the heat conduction equation $du/dt = \Delta u$), then $f = e^{-Lt} y$. Given the eigenvalue decomposition $L = U \Lambda U^T$, then the heat kernel $e^{-Lt} = U e^{-\Lambda t} U^T$, which is consistent with the Fourier transform on the graph.

The process of iteratively solving $df/dt = -L f$ with Euler's method is $f_{i+1} = (I - \eta L) f_i$, where $0 < \eta < 1$ is the step size. When the activation function is not considered, the iterative process of the graph neural network is $H_{k+1} = (I - \eta L) H_k \Theta_k$, where $\Theta$ is the parameter of the neural network. When $\eta = 1$, the above formula is the general GCN iterative process $H_{k+1} = WH_k \Theta_k$, where $W$ is the regularized adjacency matrix.

Compared the effect of taking different $\eta$ values in the (0,1] interval, and set $\eta$ as the reciprocal of the $L$ spectral radius in its experiments, considering When adding the self-loop, $\eta = 1/\lambda_n$, we can use the previous guess to roughly estimate the value of $\eta$ directly from the total number of edges and the total number of nodes. On the other hand, Because $\eta \in (0, 1]$, $I - \eta L = (1 - \eta) I + \eta A$, so this is also equivalent to introducing residual connection in GCN. And when the spectral radius of $\eta L$ is not greater than 1, the first-order Taylor expansion of $(I + \eta L)^{-1}$ is $I - \eta L$.

B. **Tentative POGNN that combine GCN and label propagation via subspace learning**

1) Net1 takes the result of GCN output as a low-dimensional representation of node features, and uses the [31] method to solve the weight matrix and perform the iterative process of label propagation.

2) Net2 takes the output of VGAE as a low-dimensional representation of node features, and uses the [31] method to solve the weight matrix and perform the iterative process of label propagation.

3) Net3 first trains a VGAE, the loss function = the classification error of VGAE + the error of VGAE decoding/reconstructing the original image + KL divergence, and the $\mu$ output by VGAE is used as a low-dimensional representation of node features, with [31] method solves the weight matrix and performs an iterative process of label propagation.

Using Adam optimization, learning rate=0.1, weight-decay=5e-4, dropout=0.5, hidden dim=16, and 100 iterations, the results are shown in Table [32] indicating that this method is superior to existing methods. LP in the table represents the label propagation algorithm [39] using the re-regularized adjacency matrix as the weight matrix.
TABLE I
TENTATIVE NETWORKS THAT COMBINE GCN AND LABEL PROPAGATION VIA SUBSPACE LEARNING

| Method          | GCN | Net1 | Net2 | Net3 |
|-----------------|-----|------|------|------|
| Acc             | 0.8130 | 0.8130 | 0.8210 | 0.8290 |

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