Understanding the Message Passing in Graph Neural Networks via Power Iteration

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Abstract

The mechanism of message passing in graph neural networks (GNNs) is still mysterious for the literature. No one, to our knowledge, has given another possible theoretical origin for GNNs apart from convolutional neural networks. Somewhat to our surprise, the message passing can be best understood in terms of the power iteration. By removing activation functions and layer weights of GNNs, we propose power iteration clustering (SPIC) models which are naturally interpretable and scalable. The experiment shows our models extend the existing GNNs and enhance its capability of processing random featured networks. Moreover, we demonstrate the redundancy of some state-of-the-art GNNs in designing and define a lower limit for model evaluation by randomly initializing the aggregator of message passing. All the findings in this paper push the boundaries of our understanding of neural networks.

1 Introduction

Nowadays the graph neural network (GNN) is one of the most widely used techniques for graph structured data analysis, with applications ranging from social sciences, physics, applied chemistry to biology and linguistics. In virtually every scientific field dealing with graph data, attempting with GNNs is people’s first choice to get an impression on their data. However, Just like the convolutional neural network (CNN), explaining the mechanism of GNN is a challenging task because of the complex nonlinear iterations.

Encouragingly, when removing the feature transformations from each layer, everything is becoming clear. We express the above idea as,

\[
\begin{align*}
X_1' &= ReLU[MX_{p_1}] \\
X_2' &= ReLU[MX_1'_{p_2}] \\
&\vdots \\
X_{k-1}' &= ReLU[MX_{p_{k-2}}X_{k-2}'] \\
X_k' &= MX_{k-1} \\
X &= \text{Softmax}(X_k'\omega_p)
\end{align*}
\]

\[
\begin{align*}
X_1 &= ReLU[MX] \\
X_2 &= ReLU[MX_1] \\
&\vdots \\
X_{k-1} &= ReLU[MX_{p_{k-2}}X_{k-2}] \\
X_k &= MX_{k-1} \\
X &= \text{Softmax}(X_k\omega_p)
\end{align*}
\]

(1)

where \(M\) is the aggregator, \(X\) is the graph feature, and \(\omega\) is the feature transformation matrix.

Using the fact that the aggregator \(M\) is nonnegative and the graph feature can always be transformed to be nonnegative, every node in a graph thus will always receive nonnegative information, that is to
say, ReLU is invalid. Then the above k-layer GNN can be expressed as,

\[
\begin{align*}
X'_1 &= MX \\
X'_2 &= MX'_1 \\
& \vdots \\
X'_{k-1} &= MX'_{k-2} \\
X'_k &= MX'_{k-1} \\
X &= \text{Softmax}(X'_\omega) \quad \text{yields} \quad \left\{ \begin{array}{l}
X'_k = M^kX \\
X = \text{Softmax}(X'_\omega) \end{array} \right.
\end{align*}
\]

The \(X'_k = M^kX\) is actually known as the power iteration (without normalization) [1]. When \(k\) is large enough, multiplying \(X\) repeatedly by the matrix \(M\) results in moving every column vector of \(X\) to the dominant eigenvector (the eigenvector of the largest-in-magnitude eigenvalue) of \(M\). In practice, GNN is a shallow iteration, then it actually calculates an eigenvalue-weighted linear combination of all the eigenvectors of the matrix \(M\). For simplicity, let’s prove the above propositions from one dimension perspective. First assume that the matrix \(M\) has \(n\) eigenvectors \(x_1, x_2, ..., x_n\) with corresponding eigenvalues of \(\lambda_1, \lambda_2, ..., \lambda_n\) in descending order. The \(n\) linearly independent eigenvectors form a basis for \(\mathbb{R}^n\). For a nonzero random starting vector \(v_0\), then has,

\[
v_0 = c_1x_1 + c_2x_2 + \ldots + c_nx_n, \quad c_i \neq 0
\]

Multiplying both sides of this equation by \(M\) produces,

\[
Mv_0 = c_1(Mx_1) + c_2(Mx_2) + \ldots + c_n(Mx_n) = c_1(\lambda_1x_1) + c_2(\lambda_2x_2) + \ldots + c_n(\lambda_nx_n)
\]

Repeated multiplication of both sides of this equation by \(M\) produces,

\[
M^k v_0 = c_1(\lambda_1^k x_1) + c_2(\lambda_2^k x_2) + \ldots + c_n(\lambda_n^k x_n)
\]

The importance of each dimension (eigenvector) is downweighted by (a power of) its eigenvalue. In spectral clustering, the top \(d\) eigenvectors generally define a subspace where the clusters are well-separated. That subspace of \(M^k v_0\) is somewhat clearer, if we scale the equation by the largest eigenvalue coefficient \(c_1 \lambda_1^k\),

\[
\frac{M^k v_0}{c_1 \lambda_1} = x_1 + \frac{c_2}{c_1} \left(\frac{\lambda_2}{\lambda_1}\right)^k x_2 + \ldots + \frac{c_n}{c_1} \left(\frac{\lambda_n}{\lambda_1}\right)^k x_n
\]

With increasing \(k\), some dimensions shrink quickly and even collapse. Hence, we can get some "good" dimensions and diminish the "bad" dimensions. In theory, we can approach the effective subspace by tuning \(k\).

The above fact is not new. Lin & Cohen already used it to detect communities in an unsupervised way and proposed power iteration clustering (PIC) [2], but constrained on one dimension.

When running power iteration with a vector space \(M^k[v_0|v_1|...|v_p]\), we can capture the true group structure from these varying convergence trajectory of different vector dimensions. We refer to the above idea as subspace power iteration clustering (SPIC), which presents a derived relationship with GNN.

In fact, there have been several attempts [3-9] in the literature to open the black box of the neural message passing. Paper[3] attributed the success of GNN to Laplacian smoothing, which makes the features of vertices in the same cluster similar and thus easy for clustering. Interestingly, the smoothing theory can be used to describe the power iteration. This is best illustrated in the context of spectral graph drawing.

Here, we plot a graph on one dimension, say \(x\) axis. Iteratively placing each node at the average between its old place and the centroid of its neighbors for \(k\) times can be expressed by,

\[
(I + D^{-1}A)^k x = x'
\]

where \(D\) is the degree matrix and \(A\) is the adjacency matrix.

Combining with the concept of community, where nodes interact more frequently with members of the same group than those of other groups, all nodes are thus on the way to their cluster centers. This is the geometric explanation of why power iteration works for the community detection. Note that \(I + D^{-1}A, D^{-1}A, I - D^{-1}A\) share the same eigenvectors, when \(k\) is sufficiently large, \(x\) converges
to the dominant eigenvector \(1_n \equiv (1, 1, ..., 1)^T\) of degree normalized Laplacian \(D^{-1}L\). That is to say, all the nodes are put in the same location. More information about spectral drawing can be found at [10].

The more interesting thing is that some scholars even extract a power model from GNNs but interpret it differently. Paper[4] missed the power iteration by taking \(M^kX\) as a feature pre-processing step. Paper[5] regarded \(M^k\) as the graph moment which counts the number of paths from node \(i\) to \(j\) of length \(k\).

The remaining interpretations [6-9] focus on graph structures or features, and try to identify the informative components and important node features which have a crucial role in GNN’s prediction. However, when \(M\) or \(X\) is random, if \(M^kX\) still contributes to the community detection, their interpretations may need some patches.

Overall, the contributions of our work are as follows:

1. We first point out another possible theoretical origin for GNNs apart from CNN.
2. We extend the existing GNNs and enhance its capability of processing no-feature graphs by our SPIC models.
3. We reclassify GNNs and demonstrate the redundancy of the existing models.
4. We define a lower limit for GNNs performance evaluation by random aggregators.

In the next section, we propose SPIC models to improve the existing state-of-the-art GNNs, then evaluate and compare them in section 3, where we also conduct comprehensive experiments to explore the properties of SPIC. Section 4 concludes the paper.

## 2 SPIC Models

In this section, we first reclassify the Laplacian aggregators and put forward a more general concept, then we propose our SPIC models. These models are categorized into three types according to the application of message-Laplacian eigenvalues and eigenvectors. Moreover, inspired by the statistical characterization of GAT on PPI data, we further enrich these linear models with nonlinear layers.

### 2.1 Laplacian Matrix

Lots of Laplacians are proposed, but there is no consensus in the literature as to which definition is most appropriate for message passing. We classify them according to the eigenvectors, since we know the mechanism of GNN.

\[
\text{Laplacian Aggregator} = \begin{cases} 
L^{sm} \equiv \{I \pm D^{-\frac{1}{2}}AD^{-\frac{1}{2}}, D^{-\frac{1}{2}}AD^{-\frac{1}{2}}\} \\
L^{rw} \equiv \{I \pm D^{-1}A, D^{-1}A\} \\
L^{di} \equiv (\Gamma + \Gamma^T)/2 
\end{cases}
\]

where \(L^{sm}\) and \(L^{rw}\) denote symmetric and random-walk Laplacian respectively. \(L^{rw}\) is similar to \(L^{sm}\) correspondingly, \(L^{rw} = I - D^{-\frac{1}{2}}(I - L^{sm}D^{-\frac{1}{2}})\). \(L^{di}\) is directed Laplacian [11] and \(\Gamma\) is an asymmetric weight matrix.

Moreover, we denote \(L^G\) as the generalized message Laplacian, by which passing messages contributes to the community detection. In this paper, we treat the superscript and subscript notations as the same.

### 2.2 Static Laplacian SPIC

We propose SPIC models for some state-of-the-art GNNs to show the idea of Static Laplacian. GNNs are listed in table 1, where \(A = A + I\), \(\bar{D}_{ii} = \sum_{j=0} A_{ij}\), \(\omega^\prime\) is the weight matrix in each GNN layer and \(\omega_p\) is the feature transformation in a linear model. Interestingly, the basic GCN SPIC model is already proposed and called SGC, but its theory is totally different from ours. It misses the power iteration by taking \((\bar{D}^{-\frac{1}{2}}, \bar{A}\bar{D}^{-\frac{1}{2}})^k X\) as a pre-processing step and leaves many questions, like why can we remove the activation functions from GNNs and does it always work, and is there
The SPIC model of Spectral GCN provides a new understanding on its convolutional operations.

The SPIC model of ChebNet and TAG-like algorithms is also already proposed and called APPNP.

The eigenvectors are invariant and the eigenvalues are dynamic. In essence, it calculates a learned eigenvalue-weighted linear combination of the eigenvectors at the expense of high computations.

only the model redundancy? All these questions will be answered later. We denote this model as,

\[ DAD(SGC) \equiv (\beta I + \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}})^k X_\omega \quad \beta = 0, 1, 2... \] (9)

Similarly, the linear model of GraphSAGE-mean can be written as,

\[ DA \equiv (\beta I + \tilde{D}^{-1} \tilde{A})^k X_\omega \quad \beta = 0, 1, 2... \] (10)

Static Laplacian SPIC is close to the original power iteration and uses one Laplacian matrix as the aggregator.

2.3 Semi-static Laplacian SPIC

The aggregators listed in table 2 suffers from expensive computational costs and the model redundancy. We only provide some easy comparisons in section 3 and put more focus on analysis.

The SPIC model of Spectral GCN provides a new understanding on its convolutional operations. Removing all the activation functions and the layer weights produces,

\[ X' = U g(A_0)...g(A_k) U^T X_\omega \approx U g(A)^k U^T X_\omega \] (11)

The eigenvectors are invariant and the eigenvalues are dynamic. In essence, it calculates a learned eigenvalue-weighted linear combination of the eigenvectors at the expense of high computations.

The SPIC model of ChebNet and TAG-like algorithms is also already proposed and called APPNP. It derives from PageRank, which is a kind of power method. The authors of APPNP do realize this but take it as a tool just like SGC. Let’s expand them with \( K \)

\[
\begin{align*}
  X'_{Cheb} &= [\omega_0 I + \omega_1 L_{sm} + \omega_2 L^2_{sm}] X \\
  X'_{TAG} &= [\omega_0 D^{-1} + \omega_1 L_{sm} + \omega_2 L^2_{sm} + \omega_3 L^3] X \\
  X'_{APPNP} &= [\alpha + \alpha (1 - \alpha) L_{sm} + \alpha (1 - \alpha)^2 L^2_{sm} + (1 - \alpha)^3 L^3_{sm}] X_\omega
\end{align*}
\] (12)

They use a similar aggregator, which is a linear combination of GCN or DAD(SGC) models. If they don’t outperform corresponding static models(GCN / DAD), we may say the semi-static model has redundancy.

One-dimension APPNP can make the definition of semi-static SPIC more clear. We denote the starting vector \( v_0 \) in eigenspace as \( v_0 = c_1^{(0)} x_1 + c_2^{(0)} x_2 + ... + c_n^{(0)} x_n, c_i \neq 0 \), then an APPNP of \( K \) iterations is written,

\[ X'_{APPNP} = \sum_{i=0}^{K} \left( c_1^{(i)} \lambda_1 x_1 + c_2^{(i)} \lambda_2 x_2 + ... + c_n^{(i)} \lambda_n x_n \right) = g(\lambda_1)x_1 + g(\lambda_2)x_2 + ... + g(\lambda_n)x_n \] (13)

The eigenvectors are invariant and the scaling factor \( g(\lambda) \) is a mixture of eigenvalues, which is similar with the case of Spectral GCN. And that is the key of the semi-static models.
We also design an asymmetric model by using the attention weights directly. An asymmetric matrix may not satisfy the diagonalizable condition of the original power

\[ Q = \begin{pmatrix} \beta I + P \end{pmatrix}^k X \omega_p, \quad \beta = 0, 1, 2... \]  

(4)

where \( P_{ij} = \text{softmax}(\varepsilon \cdot \cos(x_i, x_j)) \), \( \varepsilon \) is a hyperparameter and we set it to 1.0 in this paper.

GAT is an interesting method. Its attention mechanism makes the relative importance of nodes different, which transforms the undirected graph into a bidirectional network with asymmetric edge weights. An asymmetric matrix may not satisfy the diagonalizable condition of the original power iteration. We can symmetrize the attention weight by averaging the matrix and its transpose. That is the idea of directed Laplacian \( L^d \). Then we can create a SPIC model by removing all activations, layer weights as well as multi-heads, and iteratively learning with only one attention vector.

\[ P_{GAT} \equiv (\beta I + U)^k X \omega_p, \quad \beta = 0, 1, 2... \]  

(5)

where \( Q = \frac{U + U^T}{2}, U_{ij} = \frac{\exp(\text{LeakyReLU}(\alpha^T x_i || x_j))}{\sum_{i \in N(i), j \in N(j)} \exp(\text{LeakyReLU}(\alpha^T x_i || x_j))} \), and \( \alpha \) is the attention vector.

We also design an asymmetric model by using the attention weight directly,

\[ P_{GAT} \_am \equiv (\beta I + U)^k X \omega_p \]  

(6)

In the experimental part, we will further talk about the symmetry issue.

### 2.5 SPIC with Nonlinear Layers

A really interesting thing about GAT is that we can use it to infer the graph types based on the attentions learned. Li et al. [20] observed that the attention weights almost distribute uniformly on all the benchmark citation networks, regardless of the heads and layers. Meanwhile, significant differences are observed for the case of PPI. We classify the above data into linear and nonlinear types. For nonlinear data, we need to add some nonlinear layers into our SPIC models. Three testing models based on P_GAT are given,

\[ P_{GAT} \_relu1 \equiv \begin{cases} X = X \omega_p, \\ X = \text{ReLU}(QX) + \beta X, \\ X' = (\beta I + Q)^k X \omega_p. \end{cases} \]  

(7)

\[ P_{GAT} \_General \equiv \begin{cases} X^0 = X \omega_p, \\ X^k = \text{ReLU}(Q X^{k-1} \omega_p) + \beta X^{k-1}, \\ X' = X^k \omega_p. \end{cases} \]  

(8)

\[ P_{GAT} \_w \equiv \begin{cases} X = X \omega_p, \\ X' = (\beta I + Q)^k X \omega_p. \end{cases} \]  

(9)

ReLU is put on the first layer of P_GAT_\_relu to keep the features nonnegative. \( Q \) and \( X \) are all nonnegative, so everything will stay in the first quadrant during the power iteration. We put ReLU and another feature transformation \( \omega_p \) at each layer of P_GAT_General to strengthen its learning ability. P_GAT_w is designed as the linear model of P_GAT_General.

By setting \( Q = \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} \), we can propose DAD_\_relu1, DAD_General and DAD_w respectively. In section 3, we will explore the nonlinear issue by testing these models on PPI.
We focus on the task of node classification by using citation networks [21] and PPI [22] data. All experiments about GNNs are performed based on the codes released by PyTorch. Our models and training settings may be found at https://github.com/Eigenworld/SPIC.

### 3 Experiment and Exploration

In this section, we first evaluate and compare SPIC models and GNNs on citation networks, then conduct comprehensive experiments to explore the properties of SPIC, and answer all the questions stated in section 2.

#### 3.1 Datasets and Codes

We focus on the task of node classification by using citation networks [21] and PPI [22] data. All the citation networks are PyTorch built-in data, which are split well for training. For PPI, we choose 2 of its 24 networks and treat them as one big network. Dataset statistics are summarized in Table 4.

All experiments about GNNs are performed based on the codes released by PyTorch. Our models and training settings may be found at https://github.com/Eigenworld/SPIC. All the results are averaged over 10 (for semi-static) or 20 runs, 100 epochs each run in this paper.

#### 3.2 Comparison between GNNs and SPIC models

For the sake of fairness, all GNNs compute 64 hidden features and all linear models are iterated for 2 or 3 times. Table 5 shows that removing the activations and layer weights from GNNs doesn’t degrade the performance on citation networks. In fact, linear models achieve comparable performance (denoted by the bold) to state-of-the-art GNNs. The results of two linear GAT show no difference between symmetric and asymmetric aggregators. In random Laplacian part, we will further test this. TAG and APPNP suffers from the model redundancy for no superior performance than GCN and DAD.

Moreover, Paper [20] shows that the citation networks are linear structured and all GAT layers and heads learn a similar weight matrix. This may explain why all the activations and layer weights can be removed from GNNs on citation networks. Table 6 presents further tests on nonlinear data. Let’s first observe attention weights of GAT in Fig.1, where different layers and heads capture different attentions. Pure linear models don’t work this time. While adding ReLU to the first iteration, DAD_relu1 behaves closely to GAT. When adding the activation and layer weight to each iteration,

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**Table 4: Dataset statistics of the citation networks and PPI**

| Type  | Dataset  | #Nodes | #Edges | Train/Val/Test | Connected |
|-------|----------|--------|--------|----------------|-----------|
| Linear| Cora     | 2,708  | 5,429  | 140/500/1000   | No        |
| Linear| Citeseer | 3,327  | 4,732  | 120/500/1000   | No        |
| Linear| Pubmed   | 19,717 | 44,338 | 60/500/1000    | Yes       |
| Nonlinear| PPI   | 2,599  | 27,189 | 2050/297/252   | No        |

**Table 5: Test accuracy (%) on citation networks**

| Model       | Cora       | Citeseer   | PubMed     |
|-------------|------------|------------|------------|
| GCN         | 82.2 ± 0.6%| 82.3 ± 0.5%| 72.0 ± 1.1%| 72.0 ± 0.4%| 78.8 ± 0.5%| 79.2 ± 0.4%|
| SAGE DA     | 82.3 ± 0.9%| 82.3 ± 0.5%| 71.4 ± 1.0%| 72.3 ± 0.2%| 78.5 ± 0.5%| 79.3 ± 0.7%|
| AGNN P_AGN   | 81.5 ± 0.7%| 82.5 ± 0.6%| 71.5 ± 0.7%| 72.5 ± 0.5%| 78.9 ± 0.7%| 79.0 ± 0.6%|
| GAT P_GAT    | 82.4 ± 0.8%| 81.7 ± 0.5%| 71.7 ± 0.8%| 71.2 ± 1.2%| 78.1 ± 0.6%| 77.3 ± 1.1%|
| P_GAT_am     | 81.0 ± 0.7%| 71.0 ± 0.8%| 77.3 ± 1.0%| 77.3 ± 1.0%| 77.3 ± 1.0%| 77.3 ± 1.0%|
| TAG APPNP    | 82.4 ± 0.9%| 82.4 ± 0.7%| 71.2 ± 0.9%| 72.0 ± 0.3%| 78.7 ± 0.4%| 78.8 ± 0.7%|

**Table 6: Test Micro F1 Score (%) on PPI**

| Model  | GAT         | P_GAT       | P_GAT_relu1 | P_GAT_General | P_GAT_w     |
|--------|-------------|-------------|-------------|---------------|-------------|
| PPI    | 65.5 ± 0.5% | 51.0 ± 1.0% | 54.8 ± 1.8% | 63.6 ± 0.5%   | 53.2 ± 0.8% |
| Model  | GAT         | P_GAT       | P_GAT_relu1 | P_GAT_General | P_GAT_w     |
| PPI    | 62.1 ± 0.6% | 46.1 ± 1.0% | 64.4 ± 0.5% | 64.1 ± 0.7%   | 54.1 ± 1.0% |
Figure 1: Entropy histogram plots for attention weights of GAT on PPI. Each node entropy is calculated by
$H(\{w_{ij} \parallel j \in N(i)\}) = -\sum_{j \in N(i)} w_{ij} \log w_{ij}$.

Table 7: Test accuracy (%) on reduced Cora

| Model  | Cora_800       | Cora_193       |
|--------|----------------|----------------|
| GCN    | 80.6 ± 0.5%    | 75.5 ± 1.2%    |
| DAD(SGC) | 82.0 ± 0.4%   | 79.0 ± 0.6%    |
| SAGE   | 80.9 ± 0.5%    | 76.2 ± 0.9%    |
| DA     | 81.6 ± 0.7%    | 79.2 ± 0.4%    |
| AGNN   | 80.7 ± 0.7%    | 78.5 ± 0.8%    |
| P_AGNN | 81.5 ± 0.3%    | 79.1 ± 0.5%    |
| GAT    | 80.6 ± 0.5%    | 77.4 ± 0.6%    |
| P_GAT  | 80.4 ± 0.4%    | 78.6 ± 0.8%    |

P_GAT_General almost gets back to the performance of GAT. The final contrast model shows that the
nonlinear layers really work and layer weights contribute slightly too.

3.3 Graph Feature Space Exploration

We first present the feature redundancy by respectively using Cora’s first 800 and a compressed
(linear independent) 193 dimensional features. The original feature size is 1433.

Table 7 shows that we are not losing much by reducing feature dimensions, especially for SPIC
models, which means we can further optimize the graph features. A follow-up question is how can
we design the width of the feature. We explore this issue by running DAD on random-feature graphs.
Table 8 reveals the fact that wider is not always better. This may reflect the width constriction
of GNNs. We further compare SPIC and state-of-the-art GNN models on well-designed random
citation networks in the following.

Take table 9 and 5 together, GNNs only serve the real features well, whereas SPIC models show their
superior performance. The noteworthy change here is that random features require more iterations
(k=20).

3.4 Random Laplacian

In section 2.1, we define the generalized Laplacian $L^G$ in the manner of message passing. Here, we
instantiate it with random symmetric and asymmetric models.

$$\begin{align*}
RL_{sm} &= [(H + H^T)/2 + I]X, \quad H = A * W \\
RL_{am} &= (A * W + I)X
\end{align*}$$

Table 8: Test accuracy (%) of DAD on random citation networks

| Model  | Cora_100     | Cora_300     | Cora_500     | Cora_1000    | Cora_2000    |
|--------|--------------|--------------|--------------|--------------|--------------|
| GCN    | 68.5 ± 0.6%  | 74.5 ± 0.7%  | 73.6 ± 0.3%  | 72.8 ± 0.5%  | 72.4 ± 0.5%  |
| DAD(SGC)| 42.4 ± 1.0%  | 47.0 ± 0.7%  | 48.8 ± 0.9%  | 50.9 ± 0.6%  | 49.6 ± 0.9%  |
| SAGE   | 65.7 ± 0.6%  | 67.0 ± 0.4%  | 69.0 ± 0.8%  | 72.0 ± 0.6%  | 68.8 ± 0.9%  |
Another instantiation is that we randomly initialize the attention vector $a$ of $P\_G\_T$ and propose $R\_G\_T\_am$ and $R\_G\_T\_sm$. The results in table 10 are pretty amazing, random Laplacian actually works. In this sense, if a method doesn’t outperform the random Laplacian, we may conclude it is not effective enough. The symmetry test on $P\_G\_T$ is consistent with the results in section 3.2, and $R\_G\_T\_am$ is slightly better than $R\_G\_T\_sm$. So they both work and we don’t need to worry about the symmetric or diagonalizable issue of the aggregator.

4 Conclusion

Our experiments with SPIC models show that many structures of the existing GNNs such as activation functions, layer weights and multi-aggregators may not be the must-have modules and provide strong evidence that the power iteration could serve as another possible theoretical origin of GNNs. In essence, GNNs construct a meaningful subspace by calculating an eigenvalue-weighted linear combination of the aggregator eigenvectors. Based on this finding, we further unify the spectral and spatial models and provide another classification criterion. The experiments on random featured networks refresh our impression about GNNs and push the boundaries of our understanding of neural networks. We hope this project opens the door for researches about the mechanism of CNN.

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