GENERALIZED LAPLACIAN REGULARIZED FRAMELET GCNS

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ABSTRACT

This paper introduces a novel Framelet Graph approach based on p-Laplacian GNN. The proposed two models, named p-Laplacian undecimated framelet graph convolution (pL-UFG) and generalized p-Laplacian undecimated framelet graph convolution (pL-fUFG) inherit the nature of p-Laplacian with the expressive power of multi-resolution decomposition of graph signals. The empirical study highlights the excellence performance of the pL-UFG and pL-fUFG in different graph learning tasks including node classification and signal denoising.

Index Terms— Graph Neural Networks, Graph Framelets, p-Laplacian Regularization

1. INTRODUCTION

Graph neural networks (GNNs) have demonstrated remarkable ability for graph learning tasks [17] and widely applied in many fields such as biomedical science [11], social networks [6] and recommender systems [16]. Although classic GNNs such as graph attention networks (GAT) [14] and graph convolution networks (GCN) [11] have achieved state-of-the-art results so far, they still suffer from the following issues: (1) most GNNs are only designed to perform low-pass filtering on graph signals, which may miss out more meaningful discriminative information contained in the high-frequency components [13, 18]; (2) poor performance for heterophilic graphs in which neighbouring nodes do not generally share the same label [2]; (3) the over-smoothing issue [12].

To tackle the issues, we employ a graph framelet framework together with p-Laplacian regularization [7]. This allows us to design a flexible framework for both homophilic and heterophilic graphs.

Graph framelet is a kind of wavelet that filters graph signals at multi-resolution thus providing expressive node representations. Its low-pass and high-pass filters further allows to fully explore the discriminative information in graph signals.

On the other hand, many classic GNN layers can be explained as the solution of a Laplacian regularized optimization problem [27]. Other Laplacian regularization can also be used in revised optimization problems for the purpose of denoising graph signals [22, 24]. As graph Laplacian regularizer measures the graph signal energy along edges under the $L_2$ metric, $L_p$ metric would be advantageous, given that the $L_p$ ($p < 2$) metric is more robust to high-frequency signals. Thus a higher model discriminative power is preserved. The early work [10] has demonstrated the advantage of adopting $L_1$ metric in Locality Preserving Projection. The recent paper [7] utilises a message-passing mechanism developed from a discrete regularization framework [25] and mathematically described as an approximation of a polynomial graph filter constructed on the spectral domain of p-Laplacians, which works efficiently on heterophilic graphs with noisy edges.

The p-Laplacian regularized optimization problem has no closed-form solution except for the case when $p = 2$ [25]. Thus an iterative algorithm is used to approximate the solution [26] and each iteration of the algorithm can be interpreted as a GNN layer [24]. As a result, we can relate this to the implicit layer approach [21], which has the potential to prevent over-smoothing issues where the node feature is re-injected at each iteration step [3].

To reap the benefits of p-Laplacian regularization in framelet domains while avoiding over-smoothing, we propose two p-Laplacian Regularized Framelet GCN models, named p-Laplacian Undecimated Framelet GNN (pL-UFG) and p-Laplacian Fourier Undecimated Framelet GNN (pL-fUFG). In such models, the p-Laplacian regularization can be either applied on the framelet domain or the reputed framelet Fourier domain [23]. It has been recently proved in [9] that the separate modelling of multi-frequency components can avoid over-smoothing and enhance the performance on heterophilic graphs. Hence, the combination of reserved high-pass and low-pass components of graph signals can benefit the subsequent graph learning tasks. The experimental results on real-world graph datasets emphasise that pL-UFG and pL-fUFG achieve regularization goals and perform satisfactorily on both homophilic and heterophilic graphs. Our contributions can be summarized in four-fold below:

(i) We define two types of new GNN layers by introducing the p-Laplacian regularizers for both decomposed and reconstructed framelets. This paves the way of introducing
more general Bregman divergence regularization in the graph framelet framework;

(ii) We initiate an iterative algorithm to solve the proposed models, and explore an alternative algorithm developed from the F-norm LPP;

(iii) We are the first to explore the possibility of applying the framelet transform for directed graphs, under the assumption of Chebyshev polynomial approximation; and

(iv) We investigate the performance of the new models on graph learning tasks for both homophilic (undirected) graphs and particularly heterophilic (directed) graphs. The experiment findings illustrate that pL-UFG and pL-iUFG are effective at real-world node classification tasks with strong robustness.

2. PRELIMINARIES

Graph. Let \( G = (\mathcal{V}, \mathcal{E}, \mathbf{W}) \) denote an undirected/directed weighted graph, where \( \mathcal{V} = \{v_1, v_2, \cdots, v_N\} \) and \( \mathcal{E} \subseteq \mathcal{V} \times \mathcal{V} \) represent the node set and the edge set, respectively, and \( \mathbf{W} = [w_{ij}] \in \mathbb{R}^{N \times N} \) is the weight matrix on edges. Further let \( \mathbf{D} = \text{diag}(d_1, \ldots, d_N) \) denote the diagonal degree matrix with \( d_i = \sum_{j=1}^{N} w_{ij}. \) The normalized graph Laplacian is defined as \( \mathbf{L} = \mathbf{I} - \mathbf{D}^{-\frac{1}{2}} \mathbf{W} \mathbf{D}^{-\frac{1}{2}}. \)

Homophily and Heterophily [7]. The homophily or heterophily of a network is used to define the relationship between labels \( \{y_i\} \) of connected nodes. The level of homophily of a graph can be measured by \( \mathcal{H}(\mathcal{G}) = \mathbb{E}_{v \in \mathcal{V}}[|\{j \in \mathcal{N}_v, y_j = y_i \}|/|\mathcal{N}_v|] \) where \( \mathcal{N}_v \) is the set of neighbors of \( v \) that share the same label as \( v \) which is the known as graph Dirichlet energy [25]. Now we propose the following generalized p-Laplacian regularizer adduced in [7], we propose a generalized p-Laplacian regularizer to define new GNN layers.

To see this, denote the rows of node embedding \( \mathbf{F} \) by \( f_i, (i = 1, 2, \ldots, N) \) in column shape, and \( \Delta_{ij} = -\delta_{ij} = \sqrt{\frac{w_{ij}}{d_i}} f_j - \sqrt{\frac{w_{ij}}{d_i}} f_i. \) Note that \( \text{tr}(\mathbf{F}^T \mathbf{L} \mathbf{F}) = \sum_{(v_i, v_j) \in \mathcal{E}} \|\Delta_{ij}\|_2^2 \) which is the known as graph Dirichlet energy [25]. Now we propose the following generalized p-Laplacian regularizer:

\[
S_p^\phi(\mathbf{F}) = \frac{1}{2} \sum_{v_i \in \mathcal{V}} \phi(\|\nabla_W \mathbf{F}(v_i)\|_p)
\]

where \( \nabla_W \mathbf{F}(v_i) = (\|\Delta_{ij}\|_2)_{v_j \in \mathcal{N}_v, v_j \in \mathcal{E}} \) and a penalty positive function \( \phi. \) For example, when \( \phi(\xi) = \xi^p \), we restore the p-Laplacian regularizer [7]. If \( \phi(\xi) = \sqrt{\xi^2 + \epsilon^2 - \epsilon} \) as an approximation to the case of \( p = 1 \), it is referred as the regularized total variation. Finally the proposed optimization problem becomes

\[
\mathbf{F} = \arg\min_{\mathbf{F}} \left\{ \mu \|\mathbf{X} - \mathbf{F}\|_F^2 + S_p^\phi(\mathbf{F}) \right\}.
\]

3. THE PROPOSED MODELS

3.1. Regularized Graph Neural Network

The first paper to explain GNN layer as a regularized signal smoothing process is [27] in which the classic GNN layers are interpreted as the solution to the regularized optimization problems, with certain approximation strategies to avoid matrix inverse in the closed-form solution. Inspired by the recent p-Laplacian regularizer adduced in [7], we propose a generalized p-Laplacian regularizer to define new GNN layers.

To see this, denote the rows of node embedding \( \mathbf{F} \) by \( f_i, (i = 1, 2, \ldots, N) \) in column shape, and \( \Delta_{ij} = -\delta_{ij} = \sqrt{\frac{w_{ij}}{d_i}} f_j - \sqrt{\frac{w_{ij}}{d_i}} f_i. \) Note that \( \text{tr}(\mathbf{F}^T \mathbf{L} \mathbf{F}) = \sum_{(v_i, v_j) \in \mathcal{E}} \|\Delta_{ij}\|_2^2 \) which is the known as graph Dirichlet energy [25]. Now we propose the following generalized p-Laplacian regularizer

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\]

3.2. p-Laplacian Framelet GNN Layers

For a graph signal \( \mathbf{X} \), the framelet (graph) convolution similar to the spectral graph convolution can be defined as

\[
\mathbf{F} = \mathbf{W}^T (\text{diag}(\theta))(\mathbf{W} \mathbf{X})
\]
where \( \theta \) is the learnable filter. We also call \( WVX \) the framelet coefficients of \( X \). The signal will then be filtered in its spectral domain according to the learnable framelet filter \( \theta \).

**p-Laplacian Undecimated Framelet GNN (pL-UFG):** Instead of simply performing the convolution each layer as in [6], we apply the p-Laplacian regularization on the framelet reconstructed signal by solving the following optimization problem to compute the layer output,

\[
F = \arg \min_{F} S_{p}^{\phi}(F) + \mu \| F - WV \|_F^2, \tag{7}
\]

where \( \mu \in (0, \infty) \). The meaning is that the layer output \( F \) is \( S_{p}^{\phi} \)-regularized signal which is sufficiently approximating the framelet filtered signal, balanced by the hyperparameter \( \mu \).

One possible variant to model (7) is to apply the regularization individually on the reconstruction at each scale level. That is, for all the \( k, \ell \), define

\[
F_{k,\ell} = \arg \min_{F_{k,\ell}} S_{p}^{\phi}(F_{k,\ell}) + \mu \| F_{k,\ell} - \mathcal{W}_{k,\ell} \|_F \| W_{k,\ell} F_{k,\ell} \|^2. \tag{8}
\]

Such a strategy promotes different levels of signal smoothing for different frequencies and scales, a feature often preferred to have particularly for heterophilic graphs. In our experiments, we also note that the model (8) performs better than model (7).

**p-Laplacian Fourier Undecimated Framelet GNN (pL-fUFG):** In the above pL-UFG, we take a strategy of regularizing the framelet reconstructed signal. Similarly we propose the following optimization problem in their Fourier domains:

\[
F_{k,\ell} = \mathcal{W}_{k,\ell}^T F_{k,\ell} + \sum_{k=1}^{K} \sum_{\ell=0}^{L} \mathcal{W}_{k,\ell}^T F_{k,\ell}. \tag{9}
\]

where the reconstruction takes place after signals are smoothed.

### 3.3. The Algorithm

Each of optimization problems (7)-(9) can be converted into the following problem

\[
F = \arg \min_{F} S_{p}^{\phi}(F) + \mu \| F - Y \|_F^2. \tag{10}
\]

which can be solved by the following algorithm. For a given function \( \phi(\xi) \), define

\[
M_{i,j} = \frac{w_{ij}}{2} \left[ \frac{\phi'(\| \mathcal{W} F(v_i) \|_p)}{\| \mathcal{W} F(v_i) \|_p^2} + \frac{\phi'(\| \mathcal{W} F(v_j) \|_p)}{\| \mathcal{W} F(v_j) \|_p^2} \right] \| \Delta_{i,j} \|_2^{p-2}
\]

\[
\alpha_i = 1/ \left( \sum_{v_j \sim v_i} M_{i,j} + 2\mu \right), \quad \beta_i = 2\mu \alpha_i
\]

and the matrices \( M = [M_{ij}] \), \( \alpha = [\alpha_1, ..., \alpha_N] \) and \( \beta = [\beta_1, ..., \beta_N] \). Then the solution to problem (10) can be solved by the following message passing process

\[
F^{(t+1)} = \alpha^{(t)} D^{-1/2} M^{(t)} D^{-1/2} F^{(t)} + \beta^{(t)} Y \tag{11}
\]

with an initial value, e.g., \( F^{(0)} = X \). Here \( \alpha^{(t)} \) and \( \beta^{(t)} \) are calculated according to the current features \( F^{(t)} \). Specifically in experiments, we take \( \phi(\xi) = \xi^p \) and iterate (11) \( T \) times after 10 warm-up steps. We note that the existence of the residual term \( \beta^{(t)} Y \) in the above equation has been proved to prevent model from over-smoothing [3].

### 4. EXPERIMENTS

In this section, we perform empirical study for pL-UFG and pL-fUFG on real world node classification tasks with both heterogeneous and homophilic graphs. We also test the robustness of the proposed models against noises. Due to the space limitation, we report more detailed experiment results including more datasets, noise robustness and parameter tuning in [https://anonymous.4open.science/r/pL-UFG-4095](https://anonymous.4open.science/r/pL-UFG-4095).

#### Datasets

We use both homophilic and heterophilic graphs from [https://www.pyg.org/](https://www.pyg.org/) to assess pL-UFG and pL-fUFG. They are benchmark heterophilic datasets: Wisconsin, Texas, Cornell, and homophilic datasets: Cora, CiteSeer, PubMed. In our experiments, homophilic graphs are undirected and heterophilic graphs are directed (where we observe an improved performance when direction information is provided). The ratio of training, validation, and testing sets are shown in Table [1].

| Datasets       | #Class | #Feature | #Node | #Edge | H(G)    |
|----------------|--------|----------|-------|-------|---------|
| Cora           | 7      | 1433     | 2708  | 5278  | 0.825   |
| CiteSeer       | 6      | 3703     | 3327  | 4552  | 0.717   |
| PubMed         | 3      | 500      | 19717 | 44324 | 0.792   |
| Wisconsin      | 5      | 251      | 499   | 1703  | 0.150   |
| Texas          | 5      | 1703     | 183   | 279   | 0.097   |
| Cornell        | 5      | 1703     | 183   | 277   | 0.386   |

Table 1. Dataset statistics. For homophilic graphs, the training, validation and testing ratios are 20% 10% and 70%, while 60% 20% and 20% for heterophilic graphs.

#### Baseline models

We consider eight models to make a comparison with our results. These models are MLP, GCN [11], SGC [15], GAT [14], JKNet [19], APPNP [9], GPRGNN [8] and pGNN [7]. In order to evaluate the efficacy of pL-UFG and pL-fUFG models, we also utilise UFG [23] as a baseline. In our experiments, for directed graphs, UFG is implemented by using the same formula based on the Chebyshev approximation of UFG transformation matrices [2, 4], while the algorithm of optimizing \( S_{p}^{\phi} \) can be similarly derived for directed graphs.

#### Hyperparameter tuning

We use grid search for tuning hyperparameters. We test \( p \in \{1.0, 1.5, 2.0, 2.5\} \) for PGNN, pL-
**Table 2.** Test accuracy (%) of homophilic undirected graph.

| Method   | Cora       | Citeseer   | PubMed    |
|----------|------------|------------|-----------|
| MLP      | 86.04 ± 1.11 | 68.99 ± 0.48 | 82.03 ± 0.24 |
| GCN      | 84.72 ± 0.38  | 75.04 ± 1.46 | 83.19 ± 0.13  |
| SGC      | 83.79 ± 0.37  | 73.52 ± 0.89 | 75.92 ± 0.26  |
| GAT      | 84.37 ± 1.13  | 74.80 ± 1.00 | 83.92 ± 0.28  |
| JKNet    | 83.69 ± 0.71  | 74.49 ± 0.74 | 82.59 ± 0.54  |
| APPNP    | 83.69 ± 0.71  | 75.84 ± 0.64 | 80.42 ± 0.29  |
| GPGNN    | 83.79 ± 0.93  | 75.94 ± 0.65 | 82.22 ± 0.25  |
| UFG      | 80.64 ± 0.74  | 73.30 ± 0.19 | 81.52 ± 0.80  |
| PGNN     | 84.74 ± 0.67  | 75.62 ± 1.07 | 84.48 ± 0.21  |
| (Best PGNNS) | (p = 2.0) | (p = 2.0) | (p = 1.5) |

- UFG and pL-fUFG. The learning rate is chosen from {0.01, 0.005}. We consider the iteration number of p-Laplacian message passing \( T \in \{4, 5\} \) after 10 warm-up steps. For homophilic datasets we tune \( \mu \in \{0.1, 0.5, 1, 5, 10\} \) and for heterophilic graphs \( \mu \in \{3, 5, 10, 20, 30, 50, 70\} \). The framelet type is fixed as Linear (see [20]) and the level \( L \) is set to 1. The dilation scale \( s \in \{1, 1.5, 2, 3, 6\} \), and we tuned \( n \), the degree of Chebyshev polynomial approximation to all \( g \)'s in [2], [4], [2, 3, 7]. The number of epochs is set to 200, same as the baseline model [7].

**Experiment analysis.** Table 2 summarizes the results on homophilic datasets. The values after ± are standard deviations. The top three results are highlighted in **First, Second, and Third.** From our experiment, pL-UFG and pL-fUFG can achieve superior performance. When \( p = 1 \), pGNN, pL-UFG, and pL-fUFG only work on some specific graphs since the output of the graph gradient will be a step function which may result in uncertainty of the output [4], due to non-differentiable objectives. During the experiment, we discover that while setting the trade-off term \( \mu \) for pL-UFG and pL-fUFG, the value of \( \mu \) is significantly higher than pGNN, indicating that the framelet has a major impact on the performance of the model. The findings of pL-UFG and pL-fUFG on heterophilic graphs are shown in Table 3. pL-UFG and pL-fUFG both can outperform MLP and other state-of-the-art GNNs under a low homophilic rate and obtain superior performance. In terms of denoising capacity, pL-UFG and pL-fUFG fared better than the baseline models. Finally, we conducted denoising experiments compared with PGNNS. Figure 1 illustrates both pL-UFG and pL-fUFG outperform other models.

**Discussion for \( p < 2 \).** Comparing \( p < 2 \) with \( p = 2 \) (known as Dirichlet energy regularization), we note that the case of \( p < 2 \) imposes lesser penalty for large gradient \( \nabla_W F \) than \( p = 2 \). Thus, the local variation is preserved, ensuring better model discriminative power (particularly for heterophilic graphs). The framelets utilise the retained local variation (from \( p < 2 \)) as high-frequency node information so that the over-smoothing is avoided. This also can explain the results in Table 3. Node classification for heterophilic graphs where the nodes have a great level of variation, benefits from the retained high-frequency information from the proposed models.

5. **CONCLUSION AND FURTHER WORK**

This paper introduces a novel framelet graph approach based on p-Laplacian GNN. The p-Laplacian regularization provides a great flexibility to make framelet adaptive to both homophilic undirected and heterophilic directed graphs and therefore largely enhance model’s discriminative and predictive power. This is verified by extensive numerical experiments where our proposed model outperforms baselines on various types of graph datasets. In addition, the proposed model is robust to noise perturbation, even when the noise level is high. The positive results show the great potential and encourage further exploration. Our future study includes developing an adaptive p-Laplacian regularization scheme separately on both low and high frequency spectral domains.
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