SLOG: An Inductive Spectral Graph Neural Network Beyond Polynomial Filter

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Abstract

Graph neural networks (GNNs) have exhibited superb power in many graph related tasks. Existing GNNs can be categorized into spatial GNNs and spectral GNNs. The spatial GNNs primarily capture the local information around each node, while the spectral GNNs are able to operate on the frequency signals of the entire graph. However, most, if not all, existing spectral GNNs are faced with two limitations: (1) the *polynomial limitation* that for most spectral GNNs, the expressive power in the spectral domain is limited to polynomial filters; and (2) the *transductive limitation* that for the node-level task, most spectral GNNs can only be applied on relatively small-scale graphs in transductive setting. In this paper, we propose a novel spectral graph neural network named SLOG to solve the above two limitations. For the *polynomial limitation*, SLOG proposes a novel filter with real-valued order with geometric interpretability, mathematical feasibility and adaptive filtering ability to go beyond polynomial. For the *transductive limitation*, SLOG combines the subgraph sampling technique in spatial GNNs and the signal processing technique in spectral GNNs together to make itself tailored to the inductive node-level tasks on large-scale graphs. Extensive experimental results on 16 datasets demonstrate the superiority of SLOG in inductive homophilic and heterophilic node classification task.

1. Introduction

In the era of big data and AI (Ban et al., 2021; 2023; Wei et al., 2023; Liu et al., 2020a;b; Roach et al., 2020; Du et al., 2021; Lin et al., 2024; Wei et al., 2024), graph neural networks (Hamilton et al., 2017; Veličković et al., 2018) (GNNs) have demonstrated strong learning ability on graph related tasks such as node classification (Kipf & Welling, 2016; Wu et al., 2019; He et al., 2021; Yan et al., 2022a; Liu et al., 2023; Fu et al., 2024), link prediction (Zhang & Chen, 2018; Yan et al., 2024a;b; Wang et al., 2023a), network alignment (Yan et al., 2021a;b; 2022b; Zeng et al., 2023a; 2024), node clustering (Fu et al., 2020; Jing et al., 2022; 2024; Li et al., 2022a; Zeng et al., 2023b; Fu et al., 2023) and knowledge graph reasoning (Wang et al., 2018; Vashishth et al., 2019; Liu et al., 2021; 2022; Wang et al., 2022; 2023b).

Most of existing GNNs can be divided into two main categories: spatial GNNs and spectral GNNs. The spatial GNNs are designed based on the *subgraph sampling technique* and the message-passing mechanism in the spatial domain.[1] The spatial GNNs *sample* the *local topological information* around each node. For example, GraphSAGE (Hamilton et al., 2017) samples a two-hop subgraph around the target node for message-passing and obtains the embedding for the node. GAT (Veličković et al., 2018) adopts the self-attention technique to assign different weights to different edges in the sampled subgraph. Different from the spatial GNNs focusing on capturing the local information around each node, the spectral GNNs pay more attention to the frequency signals of the whole graph. Most spectral GNNs are developed based on the *graph signal processing technique* (Wang & Zhang, 2022) in the spectral domain, which can capture different frequency signals of the graph. To name a few, ChebNet (Defferrard et al., 2016) utilizes a Chebyshev polynomial filter, GNN-LF/HF (Zhu et al., 2021b) embraces a rational function, and BernNet (He et al., 2021) applies Bernstein polynomials as the filter.

However, most, if not all, existing spectral GNNs are faced with with two limitations: the *polynomial limitation* and the *transductive limitation*. Specifically, the *polynomial limitation* means that for most spectral GNNs, the expressive power in the spectral domain is limited to polynomial filters, i.e., the orders of the filters are integer-valued.[2] The order

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[1]Dealing with small-scale graphs, the spatial GNNs may directly aggregate node information from all neighbors, which can also be seen as a full neighborhood sampling.

[2]The filters in GNN-LF/HF (Zhu et al., 2021b), ARMA (Bianchi et al., 2021), CayleyNet (Levie et al., 2018), and so

of the polynomial filters, with the only exception of (Yan et al., 2023), needs to be fixed as a hyper-parameter before training and lacks flexibility. For the *transductive limitation*, it refers to the fact (Kipf & Welling, 2016; Liu et al., 2022; Yan et al., 2023) that in terms of node-level tasks, most spectral GNNs can only be applied to the transductive setting on relatively small-scale graphs and can not accommodate to the inductive setting in real-world large-scale graphs, where new nodes keep emerging. This is because these existing spectral GNNs have to precompute the graph signal processing operators such as multiplication on the adjacency matrix of the entire graph.

To address the above two limitations of existing spectral GNNs, in this paper, we propose a novel model named SLOG with three sub-models with different components/layers: SLOG(B) (Base), SLOG(N) (Nolinear), and SLOG(L) (Local). The key idea of SLOG(B) is two-fold: firstly, to solve the *polynomial limitation*, SLOG(B) proposes a novel filter with real-valued order to go beyond polynomial. In detail, we elucidate that the filter with real-valued order of SLOG(B) enjoys (1) good geometric interpretability in spatial domain; (2) mathematical feasibility in spectral domain; and (3) adaptive filtering ability for different frequency signals (e.g., low/high/band-pass and band-stop) (Section 3.1). Secondly, to resolve the *transductive limitation*, SLOG(B) creatively combines the subgraph sampling technique in spatial GNNs and the signal processing technique in spectral GNNs together, which renders SLOG(B) the inductive ability on large-scale graphs (Section 3.2). Since SLOG(B) only has one linear layer filter, we further propose two sub-models: SLOG(N) and SLOG(L). SLOG(N) extends SLOG(B) to multiple layers and adds more non-linearity into the model (Section 3.2) and SLOG(L) interpolates the global uniform filter in SLOG(B) with local adaptive filter for each subgraph (Section 3.3). Through extensive empirical evaluations on 16 real-world datasets in the node classification task, we corroborate the effectiveness of the proposed SLOG. To summarize, our contributions are three-fold:

- **Insight.** The key idea of our paper is two-fold: (1) designing a real-valued order filter with geometric interpretability, mathematical feasibility and adaptive filtering ability; and (2) combining the subgraph sampling technique in spatial GNNs and the graph signal processing technique in spectral GNNs together.
- **Model.** We propose a large-scale inductive spectral GNN beyond polynomial filter named SLOG, which includes three sub-models: SLOG(B) as the base sub-model, SLOG(N) with non-linearity and SLOG(L) for interpolating the global uniform filter in SLOG(B) with the local adaptive filter for each subgraph. While the three sub-models are differentiated by unique components/layers, they belong to the unified SLOG model.
- **Experiments.** We conduct extensive experiments on 16 datasets and empirically find that the proposed SLOG achieves comparable or better performance than the state-of-the-arts in the inductive homophilic and heterophilic node classification task, which demonstrates the superiority of SLOG.

on, are still built upon polynomial filters.

2. Preliminaries

Notations. We utilize bold uppercase letters for matrices (e.g., $\mathbf{A}$), bold lowercase letters for column vectors (e.g., $\mathbf{u}$) and lowercase letters for scalars (e.g., α). We use the superscript $\top$ for the transpose of matrices and vectors (e.g., $\mathbf{A}^\top$ and $\mathbf{u}^\top$). Consider a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V} = \{v_i\}_{i=1}^n$ represents the set of n nodes, and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ denotes the set of edges. We use $\mathbf{X} \in \mathbb{R}^{n \times f}$ to represent the node features of a graph with feature dimension f. The adjacency matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is defined such that $\mathbf{A}_{ij} = 1$ if $(v_i, v_j) \in \mathcal{E}$, and $\mathbf{A}_{ij} = 0$ otherwise. The degree matrix is $\mathbf{D} = \text{diag}(\{\sum_j \mathbf{A}_{ij}\}_{i=1}^n)$. We introduce $\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}$ as the adjacency matrix augmented with self-loop for each node, where $\mathbf{I}$ is the identity matrix, and $\tilde{\mathbf{D}}$ is the degree matrix of $\tilde{\mathbf{A}}$.

Spectral Graph Theory. The graph Laplacian matrix is defined as $\mathbf{L} = \mathbf{D} - \mathbf{A}$. We use $\mathbf{L}_{\text{sym}} = \mathbf{I} - \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}$ for the symmetrically normalized graph Laplacian matrix. Let $\mathbf{L}_{\text{sym}} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$ represents the eigen-decomposition of $\mathbf{L}_{\text{sym}}$, where $\mathbf{U} = [\mathbf{u}_1, \cdots, \mathbf{u}_n]$ is the matrix of eigenvectors, and $\mathbf{\Lambda} = \text{diag}(\{\lambda_i\}_{i=1}^n)$ is the diagonal matrix of eigenvalues. The eigenvalues of $\mathbf{L}_{\text{sym}}$ are bounded by $\lambda_i \in [0, 2)$ (Chung, 1997)[3], which also applies to the eigenvalues $\{\tilde{\lambda}_i\}_{i=1}^n$ of $\tilde{\mathbf{L}}_{\text{sym}}$. In addition, applying a function $g(\cdot)$, also known as a filter, to $\mathbf{L}_{\text{sym}}$ is equivalent to applying $g(\cdot)$ to its eigenvalues (Shuman et al., 2013):

$$g(\mathbf{L}_{\text{sym}}) = \sum_{i=1}^{n} g(\lambda_i)\mathbf{u}_i\mathbf{u}_i^\top. \tag{1}$$

This is also applicable to $\tilde{\mathbf{L}}_{\text{sym}}$. For a l-th layer simplified graph convolutional network (SGC) (Wu et al., 2019) without non-linear activation function, the final node representation matrix $\mathbf{Z}$ can be formulated as:

$$\mathbf{Z} = (\mathbf{I} - \tilde{\mathbf{L}}_{\text{sym}})^l\mathbf{X}\mathbf{W}, \tag{2}$$

where $\mathbf{X}$ is the node feature matrix and $\mathbf{W}$ is the trainable parameter matrix. Here, the linear graph convolutional layer is equivalent to applying a polynomial function

[3] In this work, we only consider connected graph without bipartite components (i.e., a component which is a bipartite graph).

$g(\mathbf{L}_{\text{sym}}) = (\mathbf{I} - \mathbf{L}_{\text{sym}})^l (l \in \mathbb{N}^+)$ to the graph Laplacian matrix, functioning as a graph filter.

Graph Homophily and Heterophily. The concept of homophily/heterophily addresses the tendency of nodes to connect with others of the same or different classes/labels respectively. There are several interpretations of homophily/heterophily in existing literature, including perspectives at the edge scale (Abu-El-Haija et al., 2019; Zhu et al., 2020; Luan et al., 2021), node scale (Pei et al., 2020), and graph scale (Lim et al., 2021). This paper specifically addresses edge heterophily, defined as the proportion of edges connecting nodes of the different types relative to the total number of edges: $h(\mathcal{G}) = \frac{\left|(v_i,v_j)\in\mathcal{E}|y_i\neq y_j\right|}{|\mathcal{E}|}$, where y_i represents the type of node v_i.

3. Model

In this section, we present the details of the proposed SLOG model. We first introduce the specially designed filter with real-valued order, which is the key component of SLOG to solve the *polynomial limitation* (Section 3.1). Equipped with the filter with real-valued order, we present how the one linear layer filter base model SLOG(B) solves the *transductive limitation* by combining the subgraph sampling technique in spatial GNNs and the frequency signal processing technique in spectral GNNs together (Section 3.2). Then, we enhance the one layer linear SLOG(B) to multi-layer nonlinear SLOG(N) (Section 3.2). To handle the varying degree of heterophily across different parts of the graph[4], we further propose the SLOG(L), which interpolates the global uniform filter from SLOG(B)/SLOG(N) with the local adaptive filter for each subgraph in corresponding SLOG(LB) and SLOG(LN) (Section 3.3). Moreover, a complexity analysis can be found in Appendix A.4.

3.1. Filter Beyond Polynomial

The filter in most existing spectral GNNs (e.g., ChebNet (Defferrard et al., 2016), APPNP (Gasteiger et al., 2018), and SGC (Wu et al., 2019)) can be summarized as follows:

$$g(\mathbf{L}_{\text{sym}}) = \sum_{k=1}^{K} \alpha_k \mathbf{L}_{\text{sym}}^k, \tag{3}$$

where $\mathbf{L}_{\text{sym}}$ is the symmetrically normalized graph Laplacian and K is order of the polynomial. To map the filter in the spectral domain to the K-hop subgraph in the spatial domain, usually, the order K is a fixed positive integer hyper-parameter, which lacks flexibility and can not be optimized as a variable during the training process. Recently, TeDGCN (Yan et al., 2023) redefines the depth/layer of GNNs and successfully builds a filter with real-valued order as: $g(\mathbf{L}_{\text{sym}}) = (\mathbf{I} - \frac{1}{2}\mathbf{L}_{\text{sym}})^d$, where d is a real number and a trainable parameter. Unfortunately, this filter can only capture low/high frequency signals and is not able to function as a band-pass/band-stop filter (Balcilar et al., 2021). Furthermore, TeDGCN has to conduct the eigen-decomposition on $\mathbf{L}_{\text{sym}}$, which means that it is still faced with the *transductive limitation*.

In this subsection, we introduce the key component of SLOG: a filter with real-valued order, $\omega(\cdot)$, to go beyond the polynomial expressiveness in the spectral domain as follows:

$$\omega(\mathbf{L}_{\text{sym}}) = (\mathbf{I} - \frac{1}{2}\mathbf{L}_{\text{sym}})^p (\mathbf{I} + (\mathbf{L}_{\text{sym}} - \mathbf{I})^2)^q, \tag{4}$$

where p and q are two trainable real-valued parameters. We opt for the filter design in Eq. (4) for the following three key properties: *geometric interpretability*, *mathematical feasibility* and *adaptive filtering*:

P1. Geometric Interpretability in the Spatial Domain.

Proposition 3.1. *The* SLOG*'s filter with real-valued order, $\omega(\cdot)$, in the spectral domain can be regarded as the combination of two linear graph convolutional networks in the spatial domain: $\omega(\mathbf{L}_{sym}) = \mathbf{S}_1^p \cdot \mathbf{S}_2^q$, where $\mathbf{S}_1 = \frac{1}{2}(\mathbf{I} + \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}})$ and $\mathbf{S}_2 = \mathbf{I} + (\mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}})^2$.*

The proof can be found in Appendix A.1. Based on Proposition 3.1, the filter in Eq. (4) essentially represents the combination of two linear graph convolutional networks with trainable real-valued depths, which is composed of a series of operations applied to the adjacency matrix $\mathbf{A}$. This process involves symmetric normalization of $\mathbf{A}$, and addition of self-loops to both one-hop and two-hop adjacency matrices.

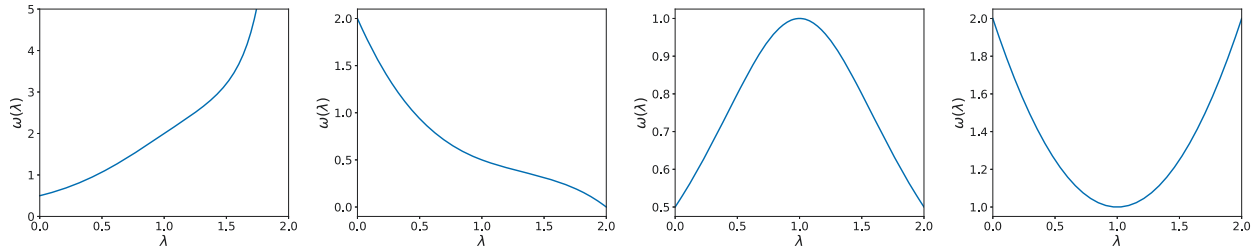
P2. Mathematical Feasibility. The eigenvalues of $\mathbf{L}_{\text{sym}}$ are confined within the range $\lambda_i \in [0, 2)$. And the filter $\omega(\mathbf{L}_{\text{sym}})$ comprises two components: $(\mathbf{I} - \frac{1}{2}\mathbf{L}_{\text{sym}})^p$ and $(\mathbf{I} + (\mathbf{L}_{\text{sym}} - \mathbf{I})^2)^q$. The first part, a polynomial function of $\mathbf{L}_{\text{sym}}$, is positive-definite, leading to the mathematical feasibility to compute its exponentiation by any real number p [5]. Likewise, the second part is also positive-definite and enjoys similar mathematical feasibility.

P3. Adaptive Filtering. The frequency response of the proposed filter under various parameter configurations is illustrated in Figure 1. This demonstrates the filter's ability to be transformed into high-pass, low-pass, band-pass, or band-stop filters by optimizing the parameters p and q in the real number domain.

Given the filter with real-valued order in Eq. (4), we next introduce the details of SLOG and how it can be applied

[4] Please refer to Figure 3 and Section 3.3 for details.

[5] For a positive-definite matrix, computing the real-valued order of the matrix is equivalent to conducting eigen-decomposition and computing the power of the eigenvalues. (Shuman et al., 2013)



(a) High pass ($p=-1, q=-1$) (b) Low pass ($p=1, q=1$) (c) Band pass ($p=0, q=-1$) (d) Band stop ($p=0, q=1$)

Figure 1. The frequency responses of the proposed filter with different parameters.

to the inductive setting and run on large-scale graphs in Section 3.2.

3.2. SLOG(B) and SLOG(N)

Algorithm 1 SLOG(B)

Input: Graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$; node feature $\mathbf{X}$; node $v \in \mathcal{V}$; hop number of subgraphs K; maximum neighbor numbers of each depth $\{N_i\}$.
Output: Vector representations $\mathbf{z}_v$ for node v.
 # Step 1: *Sampling K-hop subgraph*
$\mathcal{G}_v(\mathcal{V}_{\mathcal{G}_v}, \mathcal{E}_{\mathcal{G}_v}) \leftarrow SAMPLE(\mathcal{G}, \{v\}, K, \{N_i\})$
 # Step 2: *Calculation and Filtering*
Compute node feature $\mathbf{X}_{\mathcal{G}_v}$ and symmetrically normalized Laplacian matrix $\mathbf{L}_{\mathcal{G}_v}$ of $\mathcal{G}_v$
 # Step 3: *Obtaining node representation*
$\mathbf{Z}_{\mathcal{G}_v} \leftarrow \omega(\mathbf{L}_{\mathcal{G}_v})\mathbf{X}_{\mathcal{G}_v}\mathbf{W}$
$\mathbf{z}_v \leftarrow \mathbf{Z}_{\mathcal{G}_v}(v)$
return $\mathbf{z}_v$

 # Method: *Subgraph sampling strategy*
function $SAMPLE(\mathcal{G}, \mathcal{V}_i, K, \{N_i\})$
  $\mathcal{V}^{(0)} \leftarrow \mathcal{V}_i$
  for $k = 1$ to K **do**
    Sample $\mathcal{S}_u \subseteq \mathcal{N}(u)$, **s.t.** $|\mathcal{S}_u| \leq N_k$ for each $u \in \mathcal{V}^{(k-1)}$, where $\mathcal{N} : v \to 2^{\mathcal{V}}$ is the neighbor function of $\mathcal{G}$.
    $\mathcal{V}^{(k)} \leftarrow (\bigcup_{u \in \mathcal{V}^{(k-1)}} \mathcal{S}_u) \cup \mathcal{V}^{(k-1)}$
  end for
  return $\mathcal{G}(\mathcal{V}^{(K)}, \mathcal{E}^{(K)})$
end function

In this subsection, we present the details of SLOG(B) and SLOG(N). To handle the inductive setting and large-scale graphs, the key idea of SLOG is to integrate the *subgraph sampling technique* from spatial GNNs with the proposed filter with real-valued order in Section 3.1. In other words, for a given node v, SLOG applies the filter on a sampled subgraph centered on v, whose size is much smaller than the whole graph. In this way, SLOG fits into the inductive setting and avoids the eigen-decomposition of the whole graph, which enables it to be run on large-scale graphs.

Concretely, for a target node v, as shown in Algorithm 1, SLOG(B) contains 3 parts: (1) Firstly, we sample a subgraph $\mathcal{G}_v$ around v: starting from v, we sample a K-hop graph with random node mask. All the sampled nodes and the edges between them form the subgraph $\mathcal{G}_v$; (2) Based on $\mathcal{G}_v$, we calculate the symmetrically normalized Laplacian matrix $\mathbf{L}_{\mathcal{G}_v}$ of $\mathcal{G}_v$ and apply the filter $\omega(\cdot)$ in Eq. (4) on $\mathbf{L}_{\mathcal{G}_v}$; (3) Finally, the representations of nodes in $\mathcal{G}_v$ is obtained as follows:

$$\mathbf{Z}_{\mathcal{G}_v} = \omega(\mathbf{L}_{\mathcal{G}_v})\mathbf{X}_{\mathcal{G}_v}\mathbf{W}, \tag{5}$$

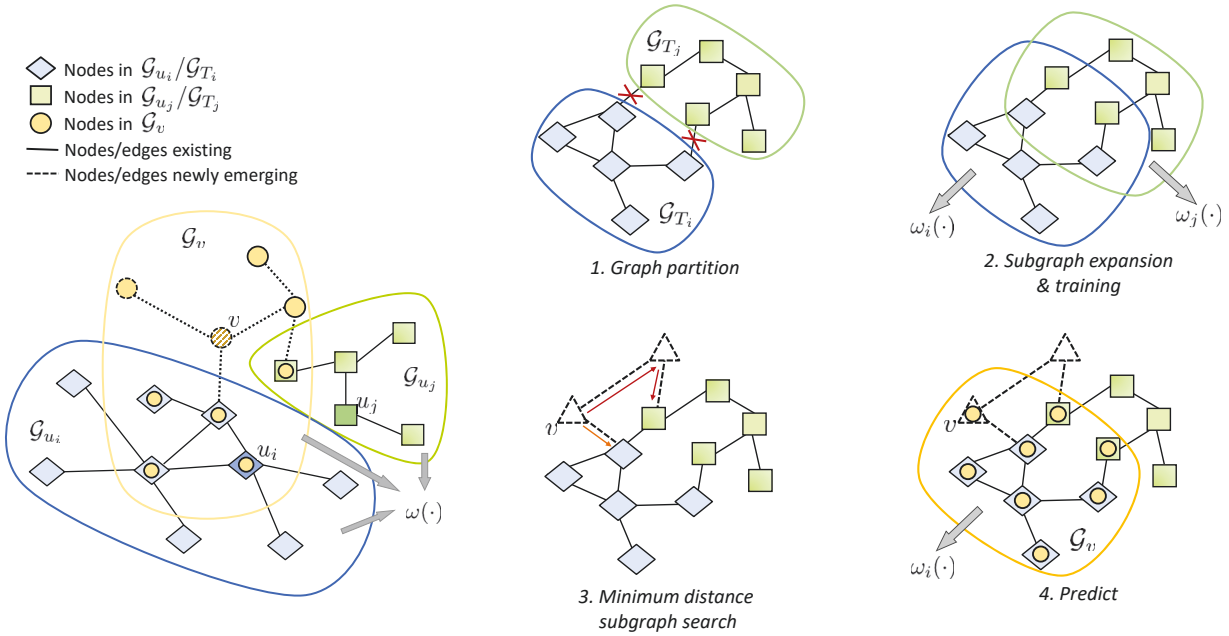
where $\mathbf{W}$ is the parameter matrix. An illustrative example of SLOG(B) is shown in Figure 2(a).

From the above introduction of SLOG(B) and the filter $\omega(\cdot)$ in Section 3.1, we can find that SLOG(B) is able to solve the *polynomial limitation* and the *transductive limitation* with the help of (1) the filter with real-valued order; and (2) the combination of the subgraph sampling technique in spatial GNNs and the frequency signal processing technique in spectral GNNs.

Nevertheless, this simple linear filter in SLOG(B) does not possess non-linearity. To address this, we further propose an enhanced sub-model, SLOG(N), which includes L layers of SLOG(B). In addition, it not only incorporates non-linear activation functions between filters but also introduces residual connections (He et al., 2016). Details of the structure are illustrated in a figure provided in Appendix A.2. The residual connections make the output become an interpolation of the embeddings from previous layer and the embeddings after transformation by Eq. (4). Specifically, in each layer, the representation matrix is updated by:

$$\mathbf{H}_{\mathcal{G}_v}^{(l)} = \sigma(\omega^{(l)}(\mathbf{L}_{\mathcal{G}_v})\mathbf{H}_{\mathcal{G}_v}^{(l-1)}\mathbf{W}_1^{(l)} + \mathbf{H}_{\mathcal{G}_v}^{(l-1)}\mathbf{W}_2^{(l)}), \tag{6}$$

where $\sigma(\cdot)$ denotes the activation function, $\omega^{(l)}(\cdot)$ denotes the filter at the l-th layer, $\mathbf{H}_{\mathcal{G}_v}^{(l)}$ is the representation matrix at the l-th layer, and $\mathbf{W}_1^{(l)}$ and $\mathbf{W}_2^{(l)}$ are the parameter matrices at the l-th layer.



(a) SLOG(B)/SLOG(N) (b) SLOG(L)

Figure 2. An overview of the proposed SLOG. (a) In SLOG(B)/SLOG(N), nodes u_i and u_j are associated with K-hop subgraphs $\mathcal{G}_{u_i}$ and $\mathcal{G}_{u_j}$ respectively. The filter with real-valued order, $\omega(\cdot)$, is applied to these subgraphs during model training. New nodes, depicted with dashed outlines, are processed similarly: sampled subgraphs are generated and the established filter is utilized for prediction. For node v, its corresponding subgraph $\mathcal{G}_v$ is employed for prediction. (b) In SLOG(L), the graph is partitioned into M subgraphs; for instance, two such subgraphs are $\mathcal{G}_{T_i}$ and $\mathcal{G}_{T_j}$. Each subgraph is expanded to restore disrupted edges, and a combination of global and respective local filters ($\omega_i(\cdot)$ for $\mathcal{G}_{T_i}$, $\omega_j(\cdot)$ for $\mathcal{G}_{T_j}$) is applied during training. Newly added nodes are assigned to the nearest subgraph, exemplified by node v being matched with $\mathcal{G}_{T_i}$, and predictions are made using the corresponding filter $\omega_i(\cdot)$.

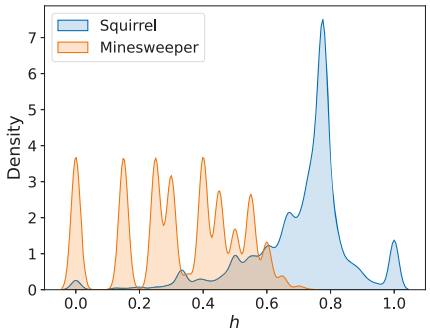


Figure 3. The one hop edge heterophily density of two real-world datasets: Squirrel (Rozemberczki et al., 2021) and Minesweeper (Platonov et al., 2023). The x-axis represents the edge heterophily (h), and the y-axis shows the corresponding density distribution. For all nodes in the graph, we sample 1-hop ego-graph for each node, and the density of the distribution can be defined as $\rho(h) = \Delta N(h)/\Delta h$, where $N(h)$ represents the proportion of the subgraphs that have an edge heterophily equal to h. The edge heterophily distribution of Squirrel is uniform, while that of Minesweeper is varying.

3.3. SLOG(L)

Actually, SLOG(B), SLOG(N), and various other heterophilic graph-oriented methods, such as GPRGNN (Chien et al., 2020), H_2GCN (Zhu et al., 2020), and BernNet (He et al., 2021) employ one single uniform filter to capture the frequency information of the whole graph. Nevertheless, heterophily in graphs is not uniformly distributed and can exhibit significant variation across different graph regions, which has been exemplified by Figure 3.

Therefore, one uniform filter with the same parameters (e.g., same p and q in Eq. (4)) for all subgraphs can not effectively capture the varying local heterophily. To address this issue, the proposed SLOG(L)'s filter contains two parts: one global uniform filter from SLOG(B)/SLOG(N) and one local adaptive filter for each subgraph, which is tailored to capture the local frequency signals. The filter for SLOG(L) is outlined in Eq. (7).

$$\omega_i(\mathbf{L}_{\mathcal{G}_v}) = (\mathbf{I} - \frac{1}{2}\mathbf{L}_{\mathcal{G}_v})^{p_i'}(\mathbf{I} + (\mathbf{L}_{\mathcal{G}_v} - \mathbf{I})^2)^{q_i'}, \quad (7)$$

where $p_i' = \beta p_{\text{glo}} + (1-\beta)p_i$ and $q_i' = \beta q_{\text{glo}} + (1-\beta)q_i$ represent the weighted combinations of global and local parameters. Here, β is a hyper-parameter that modulates the

balance between global and local filters. The parameters p_{glo} and q_{glo} are associated with the global uniform filter, while p_i and q_i are adaptive to the i-th subgraph. By interpolating the parameters of the global filter with those of the local filter, SLOG(L) can address the varying edge heterophily distribution across different subgraphs.

As illustrated in Figure 2(b), SLOG(L) contains the following steps: (1) Graph partition: when the number of nodes in the graph is extremely large, it is infeasible for SLOG(L) to adopt the same sampling strategy as SLOG(B)/SLOG(N) due to the growing number of parameters (i.e., one (p_i, q_i) for one node v_i). Thus, we employ the METIS graph partition method (Karypis & Kumar, 1998) to partition the training graph into M subgraphs, $\{\mathcal{G}_{T_i}(\mathcal{V}_{T_i}, \mathcal{E}_{T_i})\}_{i=1}^{M}$. More details about METIS are presented in Appendix C.3; (2) Subgraph expansion and training: for each subgraph $\mathcal{G}_{T_i}$, the graph partition may disrupt some edge connections, thus we augment it with nodes and edges within K-hop distance from $\mathcal{G}_{T_i}$. This process can restore the disrupted edges in $\mathcal{G}_{T_i}$. After this step, we pursue the same procedure in SLOG(B)/SLOG(N) to apply the filter $\omega_i(\cdot)$ in Eq. (7) on the subgraph. The filter $\omega_i(\cdot)$ is a combination of global and corresponding local filter. We then train the model; (3) Minimum distance subgraph search & prediction: in the inductive setting, when a new node v emerges, SLOG(L) calculates its distance to each subgraph, and finds out the nearest subgraph. The subgraph with the minimum distance and its corresponding filter are selected to obtain the representation of v, which can be used for prediction. The detailed algorithm of SLOG(L) is attached in Appendix A.3 due to the page limit.

4. Experiment

In this section, we evaluate SLOG on the semi-supervised node classification task. We first introduce the datasets, baselines and settings in Section 4.1. Next, in Section 4.2, we experiment with SLOG(B) and SLOG(N). In Section 4.3, we conduct experiments on SLOG(L). In addition, We conduct additional experiments on SLOG's adaptive filtering ability in Section 4.4. Due to the page limit, some additional experimental results are attached in Appendix: (1) ablation studies (Appendix B.1); (2) results of additional baselines (Appendix B.2); (3) experimental results on synthetic datasets (Appendix B.3); (4) a convergence study (Appendix B.4); and (5) experimental results using two alternative optimization methods (Appendix B.5).[6]

[6]Our code is available at https://github.com/Hsu1023/SLOG.

4.1. Experiment Setup

Datasets. We adopt 16 datasets for evaluation, including 13 small-scale datasets and 3 large-scale datasets. The small-scale datasets, sourced from (Kipf & Welling, 2016; Bojchevski & Günnemann, 2017; Shchur et al., 2018; Rozemberczki et al., 2021; Platonov et al., 2023), include two categories: the heterophilic datasets include Chameleon, Squirrel, Squirrel-filtered, Chameleon-filtered, Minesweeper, Tolokers, Amazon-ratings, and Questions; the homophilic datasets include Cora, Citeseer, DBLP, Coauthor-CS, and Coauthor-Physics. The large-scale datasets, sourced from (Hamilton et al., 2017; Zeng et al., 2019; Hu et al., 2020), are Flickr, Ogbn-arxiv, Reddit. These datasets are diverse, varying in scale, domain, and heterophilic/homophilic ratios. Detailed statistics of datasets are presented in Appendix C.1.

Baselines. We compare our method against 13 baselines, including (1) a non-topology method: MLP; (2) general GNN methods including GCN (Kipf & Welling, 2016), ChebNet (Defferrard et al., 2016), GraphSAGE (Hamilton et al., 2017), GAT (Veličković et al., 2018), APPNP (Gasteiger et al., 2018), SGC (Wu et al., 2019), GATv2 (Brody et al., 2021); (3) heterophilic graph oriented methods including GPRGNN (Chien et al., 2020), H_2GCN (Zhu et al., 2020), FAGCN (Bo et al., 2021), BernNet (He et al., 2021), JacobiConv (Wang & Zhang, 2022).

Settings. For small-scale datasets, we employ a random split of 60%/20%/20% for train/validation/test sets and conduct experiments in the inductive setting[7]. For large-scale datasets, we keep the same split and the same transductive/inductive setting as those used in the original papers. It is important to note that in the inductive setting, the models are not exposed to validation or test nodes during training. For evaluation, we use accuracy (ACC) with standard deviation (std) as the metric, averaging the results over 5 runs.

4.2. SLOG(B) & SLOG(N)

The performance comparison on small-scale datasets is detailed in Table 1 and Table 2. Our method demonstrates a notable superiority over all baselines in most datasets, achieving the best performance in 11 out of 13 small-scale datasets. Specifically, for *heterophilic* datasets (Table 1), our method surpasses every baseline across all datasets. This superiority is attributed to the method's capability to effectively discern the graph's heterophily, thereby flexibly adjusting its filter to capture a diverse range of frequency signals depending on the dataset. In contrast, for *homophilic* datasets (Table 2), our method shows excellence in 3 out of 5 datasets and ranks second in the remaining two. Notably,

[7]For spectral methods, we build a new Laplacian matrix $\mathbf{L}_{\text{sym}}$ when new nodes emerge in the inductive setting and inherit the old parameters from training.

Table 1. Evaluation results on heterophilic datasets in the inductive setting.

Datasets	Squirrel	Chameleon	Squirrel-filt.	Chameleon-filt.	Minesweeper	Tolokers	Amazon-ratings	Questions
MLP	0.336±0.014	0.469±0.004	0.366±0.021	0.380±0.021	0.788±0.000	0.775±0.000	0.449±0.005	**0.972±0.000**
GCN	0.374±0.007	0.532±0.012	0.329±0.020	0.411±0.031	0.788±0.000	0.784±0.001	0.420±0.002	0.970±0.000
ChebNet	0.350±0.004	0.535±0.005	0.333±0.019	0.372±0.025	0.823±0.001	0.783±0.003	0.393±0.001	0.969±0.001
GraphSAGE	0.387±0.011	0.246±0.043	0.349±0.013	0.360±0.041	0.810±0.002	0.794±0.003	0.436±0.005	0.970±0.000
GAT	0.306±0.006	0.484±0.020	0.329±0.017	0.344±0.024	0.787±0.001	0.776±0.000	0.392±0.001	0.970±0.000
APPNP	0.314±0.008	0.410±0.010	0.312±0.019	0.381±0.020	0.788±0.000	0.778±0.001	0.429±0.002	0.970±0.000
SGC	0.371±0.005	0.486±0.002	0.320±0.016	0.357±0.021	0.786±0.000	0.782±0.000	0.398±0.002	0.970±0.000
GATv2	0.310±0.006	0.468±0.009	0.350±0.013	0.394±0.026	0.788±0.002	0.775±0.001	0.394±0.002	0.970±0.000
GPRGNN	0.343±0.009	0.472±0.020	0.364±0.019	0.394±0.038	0.791±0.000	0.775±0.001	0.414±0.004	0.970±0.000
H_2GCN	0.359±0.005	0.454±0.007	0.335±0.025	0.381±0.026	0.824±0.001	0.788±0.001	0.442±0.002	0.971±0.000
FAGCN	0.332±0.008	0.412±0.026	0.350±0.030	0.369±0.027	0.789±0.001	0.784±0.002	0.433±0.009	0.970±0.000
BernNet	0.361±0.007	0.578±0.007	0.361±0.020	0.374±0.030	0.788±0.000	0.772±0.007	0.398±0.002	0.969±0.001
JacobiConv	0.221±0.017	0.309±0.015	0.295±0.012	0.348±0.035	0.788±0.000	0.704±0.100	0.355±0.010	0.877±0.176
SLOG(B)	**0.392±0.006**	**0.581±0.024**	**0.427±0.013**	0.420±0.023	0.822±0.009	0.796±0.005	0.451±0.007	**0.972±0.001**
SLOG(N)	0.355±0.010	0.520±0.022	0.376±0.025	**0.431±0.026**	**0.844±0.008**	**0.810±0.006**	**0.456±0.006**	**0.972±0.001**

Table 2. Evaluation results on homophilic datasets in the inductive setting.

Datasets	Cora	Citeseer	DBLP	Co.-CS	Co.-Phys.
MLP	0.695±0.017	0.680±0.016	0.769±0.004	0.925±0.002	0.962±0.000
GCN	0.863±0.005	0.746±0.010	0.847±0.008	0.905±0.001	0.958±0.001
ChebNet	0.804±0.004	0.740±0.009	0.840±0.000	0.640±0.001	0.958±0.000
GraphSAGE	0.835±0.005	0.724±0.010	0.840±0.003	0.907±0.002	**0.970±0.001**
GAT	0.852±0.010	0.739±0.008	0.848±0.005	0.938±0.001	0.958±0.001
APPNP	0.839±0.004	0.748±0.008	0.835±0.008	0.918±0.001	0.961±0.000
SGC	0.859±0.010	0.754±0.008	0.845±0.003	0.938±0.001	0.958±0.000
GATv2	0.863±0.008	0.741±0.012	0.845±0.006	0.905±0.001	0.959±0.001
GPRGNN	**0.874±0.010**	0.756±0.003	0.848±0.004	0.942±0.001	0.966±0.000
H_2GCN	0.815±0.004	0.757±0.010	0.840±0.001	0.940±0.001	0.966±0.000
FAGCN	0.845±0.007	0.751±0.014	0.835±0.007	0.932±0.013	0.963±0.003
BernNet	0.865±0.006	0.745±0.015	0.849±0.004	0.938±0.001	0.959±0.000
JacobiConv	0.584±0.034	0.559±0.098	0.455±0.041	0.882±0.008	0.924±0.010
SLOG(B)	0.865±0.011	**0.766±0.026**	**0.850±0.005**	0.934±0.003	0.959±0.002
SLOG(N)	0.761±0.010	0.675±0.026	0.839±0.003	**0.944±0.005**	0.966±0.001

Table 3. Evaluation results on large-scale datasets.

Datasets	Flickr	Ogbn-arxiv	Reddit
nodes	89,250	169,343	232,965
edges	899,756	1,166,243	114,615,892
setting	inductive	transductive	inductive
MLP	0.474±0.001	0.539±0.001	0.702±0.001
GraphSAGE	0.502±0.002	0.717±0.002	0.944±0.001
GAT	0.509±0.001	0.676±0.003	0.944±0.002
GATv2	0.517±0.001	0.675±0.001	0.957±0.000
GPRGNN	0.508±0.002	0.684±0.002	0.950±0.000
H_2GCN	0.516±0.002	0.677±0.000	OOM
SLOG(B)	0.509±0.001	**0.723±0.001**	0.954±0.000
SLOG(N)	**0.520±0.003**	0.719±0.002	**0.962±0.001**

in the Cora and Coauthor-Physics datasets, our method's performance is marginally lower than the best baseline, by only 1.4% and 0.4%, respectively. This underscores our method's effectiveness in homophilic datasets as well.

For large-scale dataset evaluation, results in Table 3 illustrate that our method consistently outperforms others. A notable aspect is the size of the Reddit dataset, which contains 115M edges and is significantly larger than those in most related studies. Due to the high computational cost, some baselines meet the out-of-memory (OOM) problem in our machine[8]. However, thanks to the sampling technique, our method is able to directly run on the graph, achieving the best performance, confirming its scalability to large-scale graphs. It is also important to note that these experiments adhere to the same transductive/inductive settings as used in the original papers, further evidencing our method's robustness across various settings.

In addition, it is observed that SLOG(N) outperforms SLOG(B) on numerous datasets, despite its more complex architecture and increased number of parameters. This improvement is attributed to the additional non-linearity in SLOG(N), which enhances the model's expressiveness. Moreover, the incorporation of residual connections in SLOG(N) helps preserve the node embedding from previous layer.

4.3. SLOG(L)

The SLOG(L) model, as introduced in Section 3.3, addresses varying distributions of homophily/heterophily ratios across a graph. In order to quantify the heterophily/homophily balance, we introduce a metric, locality. We sample a fixed number of nodes in the graph, obtain their 1-hop ego-graphs, and calculate the edge heterophily of these ego-graphs. The locality, defined as the standard deviation of all 1-hop ego-graphs' edge heterophily, inversely indicates the balance level of local edge heterophily across the whole graph.

As shown in Table 4, SLOG(LB)/SLOG(LN) enhances performance in datasets with high *locality* (e.g., Chameleon, Chameleon-filt., Minesweeper, Tolokers), suggesting its effectiveness in contexts with imbalanced ho-

[8]Since some spectral GNNs can not be run on such large-scale datasets, we do not include them in the comparison.

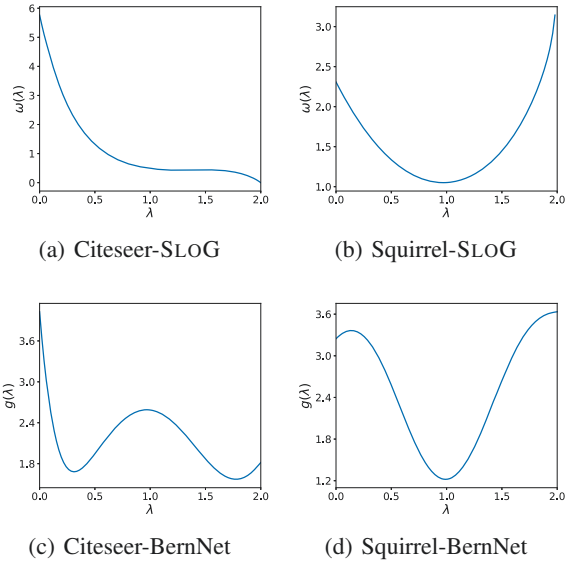
Table 4. Performance of SLOG(L) on datasets with different *locality*.

Datasets	Squirrel	Squirrel-filt.	Chameleon	Chameleon-filt.	Minesweeper	Tolokers
Locality/10^{-2}	1.85	1.66	4.16	3.03	4.08	3.84
Best of baselines	0.387±0.011	0.366±0.021	0.578±0.007	0.411±0.031	0.824±0.001	0.794±0.003
SLOG(B)	**0.392±0.006**	**0.427±0.013**	0.581±0.024	0.420±0.023	0.822±0.009	0.796±0.005
SLOG(N)	0.355±0.010	0.376±0.025	0.520±0.022	0.431±0.026	0.844±0.008	0.810±0.006
SLOG(LB)	0.387±0.008	0.409±0.010	**0.605±0.043**	0.443±0.029	0.807±0.006	0.785±0.008
SLOG(LN)	0.355±0.012	0.375±0.028	0.535±0.017	**0.453±0.041**	**0.848±0.007**	**0.814±0.004**

mophily/heterophily distributions. However, in datasets with low *locality* (e.g., Squirrel, Squirrel-filt.), the performance gain is not observed, likely due to the already balanced local edge heterophily of these graphs. Here, the addition of a local component unnecessarily complicates the model, potentially hindering the effectiveness of the model.

4.4. Adaptive Filtering to Broad Frequency Signals

In this subsection, we present the learned filters of our method on real datasets. The learned filters of our method SLOG(B) on real datasets are shown in Figure 4(a) and 4(b). To compare with BernNet, we also show the learned filters of BernNet on the same datasets in Figure 4(c) and Figure 4(d). For the homophilic Citeseer graph, SLOG(B) functions as a low-pass filter, capturing homophilic information (Figure 4(a)). Conversely, for the heterophilic Squirrel graph, it selectively filters out medium-frequency signals and preserves high-frequency ones (Figure 4(b)). However, BernNet's performance on Citeseer includes not only low-frequency signals but also some medium-frequency noise (Figure 4(c)), indicating a potential for overfitting due to its complex coefficients. Though BernNet learns filters similar to SLOG(B) on Squirrel, the fluctuating signal curves imply the capture of some extraneous signals (Figure 4(d)).



(a) Citeseer-SLOG (b) Squirrel-SLOG

(c) Citeseer-BernNet (d) Squirrel-BernNet

Figure 4. Learned filters on real dataset.

5. Related Work

Graph neural networks (GNN). GNN models can be roughly divided into two categories, i.e. spectral-based methods and spatial-based methods (Zhang et al., 2020). Spectral methods are based on the spectral graph theory, aiming to establish graph convolutional kernel in the spectral domain. The notable attempt is reported in (Bruna et al., 2013), which firstly introduces graph convolutional kernel. After that, ChebNet (Defferrard et al., 2016) utilizes Chebychev polynomials to form a convolutional kernel. GCN (Kipf & Welling, 2016) takes the first-order approximation to simplify the kernel. SGC (Wu et al., 2019) further changes multi-layer design to one linear transformation. Other spectral-based methods include (Levie et al., 2018; Li et al., 2018; Zhu et al., 2021b; Bianchi et al., 2021) and so on. Spatial-based methods mainly focus on aggregating the information of neighboring nodes. GraphSAGE (Hamilton et al., 2017) studies three different aggregators to aggregate the information of neighbors. In GAT (Veličković et al., 2018), attention mechanism is introduced as the aggregator. GIN (Xu et al., 2018) deploys MLPs to model injective functions in order to enhance the discriminative power of the GNN. We refer readers to (Zhou et al., 2020; Wu et al., 2020) for more details.

Heterophilic graph learning. While GNNs are mostly based on the homophily assumption that neighboring nodes are inclined to share the same labels, there are many real-world graphs that do not satisfy this assumption (McPherson et al., 2001). These graphs, which are called heterophilic graphs, have gained an increasing attention recently. CayleyNet (Levie et al., 2018) defines a complex Cayley filter and utilize Jacobi iteration to optimize it, while ARMA (Bianchi et al., 2021) uses auto-regressive moving average (ARMA) filter to capture the global graph structure. Geom-GCN (Pei et al., 2020) defines the geometric relationship in a latent space to use neighborhood information. FAGCN (Bo et al., 2021) utilizes the attention mechanism to seperately learn low-frequency and high-frequency signals. ACM-

GCN (Luan et al., 2021) adopts a linear combination of low/high pass filters and adaptively mix the generated node information from the two filters. CPGNN (Zhu et al., 2021a) utilizes a compatibility matrix to model the heterophilic/ homophilic relationships between nodes. TeDGCN (Yan et al., 2023) utilizes a filter with real-valued order, with its learnable parameter as the depth of graph convolutional layers, expressed as a real number. Other heterophilic graph learning methods include (Li et al., 2022b; Wang & Zhang, 2022; He et al., 2022; Zheng et al., 2023; Xu et al., 2023; Guo & Wei, 2023; Geng et al., 2023; Guo et al., 2023). We refer readers to (Zheng et al., 2022) for more details.

6. Conclusion and Limitations

In this paper, we propose an inductive spectral graph neural network named SLOG with the expressive power beyond a polynomial filter. Specifically, SLOG includes three sub-models: the base model SLOG(B), the non-linear model SLOG(N) and the local model SLOG(L). SLOG(B) is equipped with a filter with real-valued order, which enjoys geometric interpretability, mathematical feasibility and adaptive filtering. SLOG(N) adds non-linearity and residual connections into SLOG(B). To better capture the varying heterophily distribution, SLOG(L) conducts an interpolation between the global uniform filter and the local adaptive filter. Extensive experiments on 16 real-world datasets corroborate the effectiveness, scalability and robustness of SLOG in the inductive semi-supervised homophilic/heterophilic node classification task. One potential limitation of SLOG is that it only focuses on node classification problem, and we leave its extension to other tasks including link prediction as future work.

Impact Statement

This paper presents work whose goal is to advance the field of Graph Machine Learning. There are many potential societal consequences of our work, none which we feel must be specifically highlighted here.

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