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Graph Neural Networks with Diverse Spectral Filtering

   

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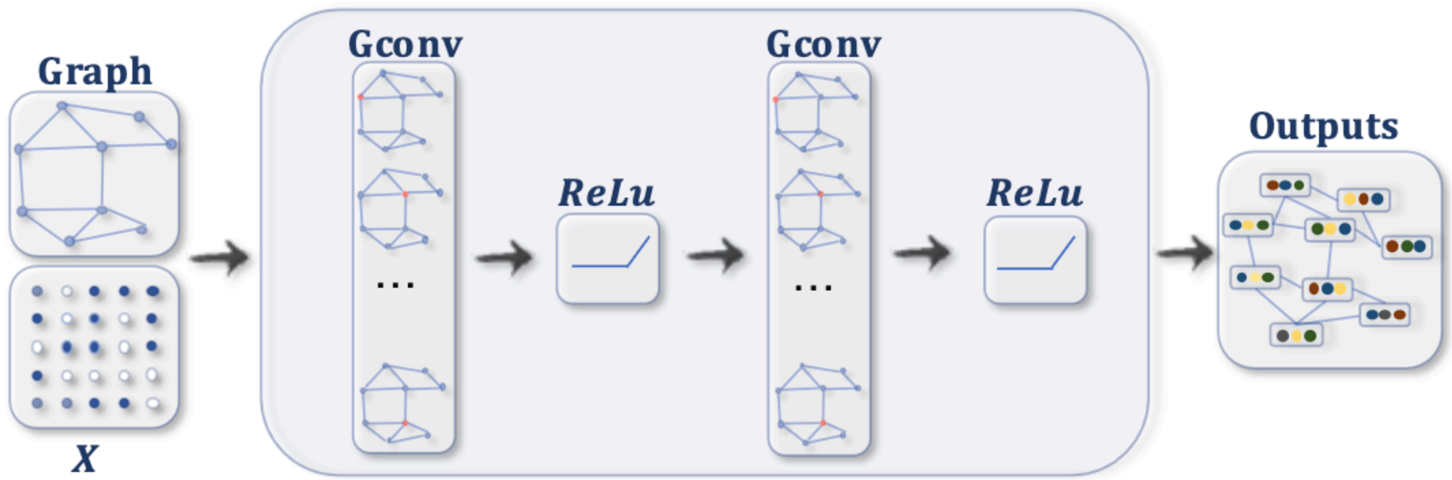
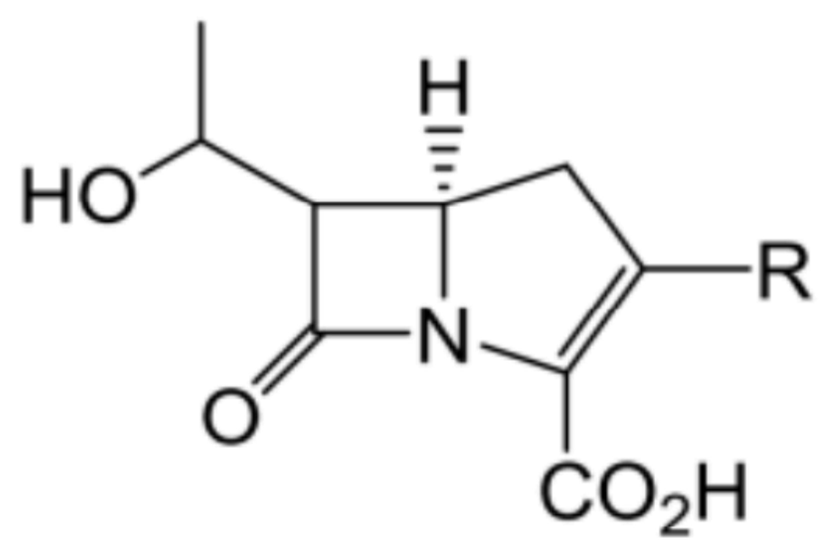
Graph Machine Learning



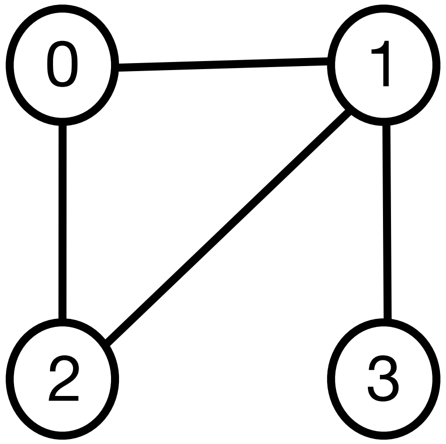
Spectral Graph Neural Networks (GNNs) apply graph convolution with polynomial spectral filters



https://web.stanford.edu/class/cs224w/slides/01-intro.pdf

Wu et al. A Comprehensive Survey on Graph Neural Networks. In TNNLS, 2020.

Spectral GNNs: Graph Fourier Transform



$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad \mathbf{D} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \mathbf{X} = \begin{pmatrix} 0 \\ 1 \\ 2 \\ 3 \end{pmatrix}$$

<u>Normalized Graph Laplacian</u>

Eigendecomposition

$$\hat{\mathbf{L}} = \mathbf{I} - \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}} = \boxed{\mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T}$$

λ_i : The i-th eigenvalue.

→ Frequency

$\mathbf{U}_i$: The i-th eigenvector.

→ Frequency Component

$$\tilde{\mathbf{X}} = \mathbf{U}^T\mathbf{X}$$

Graph Domain

Frequency Domain

$$\mathbf{X} = \mathbf{U}\tilde{\mathbf{X}}$$

Spectral GNNs: Graph Spectral Filter

Define a filter function $g : [0,2] \rightarrow \mathbb{R}$ in the frequency/spectral domain:

Fourier transform of node features → Filtering operation with frequency response → Inverse graph Fourier transform

$$\mathbf{S} = \mathbf{U}^T\mathbf{X} \qquad \tilde{\mathbf{S}}_{[i,:]} = g(\lambda_i)\mathbf{S}_{[i,:]} \qquad \mathbf{Z} = \mathbf{U}\tilde{\mathbf{S}}$$

$$\mathbf{Z} = g(\hat{\mathbf{L}}) = \mathbf{U}g(\mathbf{\Lambda})\mathbf{U}^T X$$

$$\mathbf{U}\boxed{\tilde{\mathbf{S}}} \qquad \mathbf{U}\boxed{\mathbf{S}}$$

New Coefficients   Old Coefficients

Spectral GNNs: Graph Spectral Filter

Define a filter function $g : [0,2] \rightarrow \mathbb{R}$ in the frequency/spectral domain:

Fourier transform of node features	Filtering operation with frequency response	Inverse graph Fourier transform
$\mathbf{S} = \mathbf{U}^T\mathbf{X}$	$\tilde{\mathbf{S}}_{[i,:]} = g(\lambda_i)\mathbf{S}_{[i,:]}$	$\mathbf{Z} = \mathbf{U}\tilde{\mathbf{S}}$

Take one-dimension $\mathbf{X}$ as an example:

$$\mathbf{X} = \boxed{S_1} \cdot \mathbf{U}_1 + \boxed{S_2} \cdot \mathbf{U}_2 + \cdots + \boxed{S_N} \cdot \mathbf{U}_N$$

$$\mathbf{Z} = \boxed{\tilde{S}_1} \cdot \mathbf{U}_1 + \boxed{\tilde{S}_2} \cdot \mathbf{U}_2 + \cdots + \boxed{\tilde{S}_N} \cdot \mathbf{U}_N$$

Spectral GNNs: Polynomial Approximation

Polynomial approximation to the filter function g:

$$g(\lambda) = \sum_{k=0}^{K} \omega_k \lambda^k = \sum_{k=0}^{K} \alpha_k P_k(\lambda)$$

Polynomial Basis

Fixed filter: GCN, APPNP

Learnable filter: GPR-GNN, BernNet, JacobiConv

Theoretical expressive power in learning arbitrary filter function while $K \to \infty$.

Kipf & Welling. Semi-supervised Classification with Graph Convolutional Networks. In ICLR 2017.
Klicpera et al. Predict then Propagate: Graph Neural Networks Meet Personalized PageRank. In ICLR 2019.
Chien et al. Adaptive Universal Generalized Pagerank Graph Neural Network. In ICLR 2021.
He et al. BernNet: Learning Arbitrary Graph Spectral Filters via Bernstein Approximation. In NeurIPS 2021.
Wang & Zhang. How Powerful are Spectral Graph Neural Networks. In ICML 2022.

Motivations: Homogeneous Spectral Filtering

Local modeling nature within K-hop neighborhood

$$\mathbf{Z} = \sum_{k=0}^{K} \alpha_k P_k(\hat{\mathbf{L}})\mathbf{X} \text{ while practically } \boxed{K \rightarrow \infty \Rightarrow \alpha_k \rightarrow 0}$$

All nodes share the identical transforming coefficient

$$\mathbf{Z} = \boxed{\sum_{n=1}^{N} \tilde{S}_n \cdot \mathbf{U}_n}$$

$\tilde{S}_n$ is a scalar in case of one-channel $\mathbf{X}$ as an example

Inaccurate hypothesis: homogeneous distributions between different local regions on the graph.

Chien et al. Adaptive Universal Generalized Pagerank Graph Neural Network. In ICLR 2021.
Wang & Zhang. How Powerful are Spectral Graph Neural Networks. In ICML 2022.

Motivations: Local Graph Property

Definition 1 (Local Label Homophily). We define the Local Label Homophily as a measure of the local homophily level surrounding each node v_i:

$$h_i = \frac{|\{(v_p, v_q)|\mathbf{y}_p = \mathbf{y}_q \wedge (v_p, v_q) \in \mathcal{E}_{i,k}\}|}{|\mathcal{E}_{i,k}|}$$

Here, h_i directly computes the edge homophily ratio [50] on the subgraph made up of the k-hop neighbors, and $\mathcal{E}_{i,k} = \{(v_p, v_q)|v_p, v_q \in \mathcal{N}_{i,k} \wedge (v_p, v_q) \in \mathcal{E}\}$ denotes its edge set.

Label Homophily:

$$h = \frac{|\{(v_i,v_j)|\mathbf{y}_i{=}\mathbf{y}_j \wedge (v_i,v_j) \in \mathcal{E}\}|}{|\mathcal{E}|}$$

Definition 2 (Local Graph Frequency). The Local Graph Frequency is defined by measuring the local smoothness level of the decomposed Laplacian eigenbases, and for each node v_i we have:

$$\lambda_{n,i} = \sum_{(v_p,v_q) \in \mathcal{E}_{i,k}} \left(\frac{1}{\sqrt{\deg_p}}\mathbf{u}_{n,p} - \frac{1}{\sqrt{\deg_q}}\mathbf{u}_{n,q}\right)^2$$

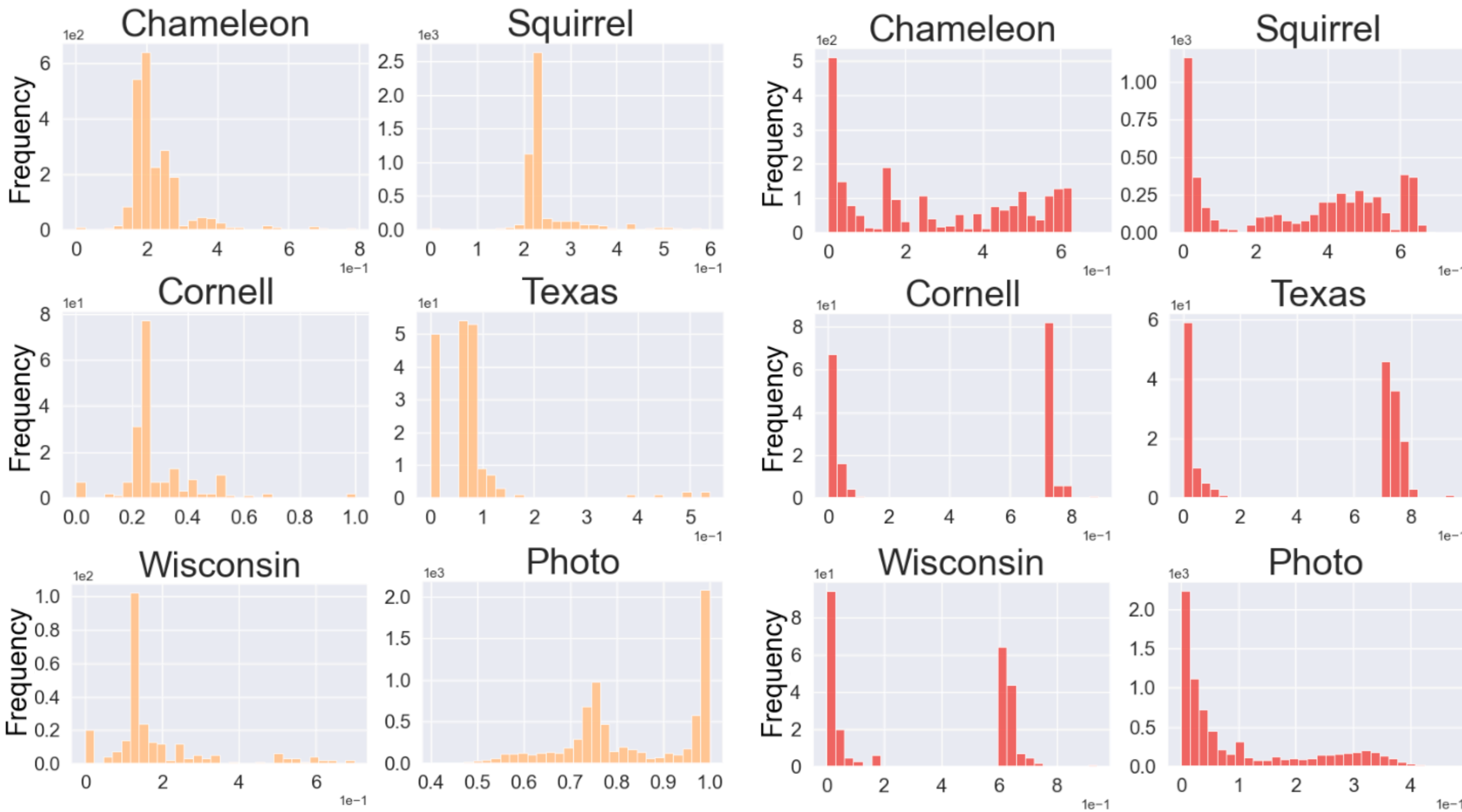
where $\lambda_{n,i}$ denotes the frequency or smoothness level of each Laplacian eigenbasis $\mathbf{u}_n$ upon the subgraph induced by the k-hop neighbors. Since all summed elements in Eq. 1 are positive and $\mathcal{E}_{i,k} \subseteq \mathcal{E}$, we can always have a $\xi_i \in (0, 1)$ such that $\lambda_{n,i} = \xi_i \lambda_n$.

Frequency (Eigenvalue):

$$\lambda_n = \mathbf{u}_n^T \hat{\mathbf{L}} \mathbf{u}_n$$

$$= \sum_{(v_p,v_q) \in \mathcal{E}} \left(\frac{1}{\sqrt{\deg_p}}\mathbf{u}_{n,p} - \frac{1}{\sqrt{\deg_q}}\mathbf{u}_{n,q}\right)^2$$

Motivations: Heterogeneous Linking Pattern



(a) Local Label Homophily **(b) Local Graph Frequency**

Evident regional heterogeneity

Our Solution: Diverse Spectral Filtering (DSF)

Homogenous spectral filtering:

$$\mathbf{Z} = \sum_{n=1}^{N} \tilde{S}_n \overset{\text{Dot product}}{\cdot} \mathbf{U}_n$$

$$\underset{\text{Scalar coefficient}}{\tilde{S}_n} = \sum_{k=0}^{K} \alpha_k P_k(\underset{\text{Graph frequency}}{\lambda_n}) \mathbf{U}_n^T \mathbf{X}$$

Diverse spectral filtering:

$$\mathbf{Z} = \sum_{n=1}^{N} \underset{\text{Vector}}{\tilde{\mathbf{S}}_n} \overset{\text{Hadamard product}}{\odot} \mathbf{U}_n$$

$$\underset{\text{The } i\text{-th element of vector coefficients}}{\tilde{\mathbf{S}}_n(i)} = \sum_{k=0}^{K} \alpha_k P_k(\underset{\text{Local graph frequency}}{\lambda_{n,i}}) \mathbf{U}_n^T \mathbf{X}$$

$\mathbf{X}$ is taken as one-dimension as an example

Our Solution: Diverse Spectral Filtering (DSF)

The calculation of $\lambda_{n,i}$ would be computationally expensive, which requires not only Laplacian decomposition but also subgraph extraction.

$\mathbf{X}$ is taken as one-dimension as an example

Our Solution: Diverse Spectral Filtering (DSF)

Substitution using $\lambda_{n,i} = \xi_i \lambda_n$ s.t. $0 < \xi_i < 1$

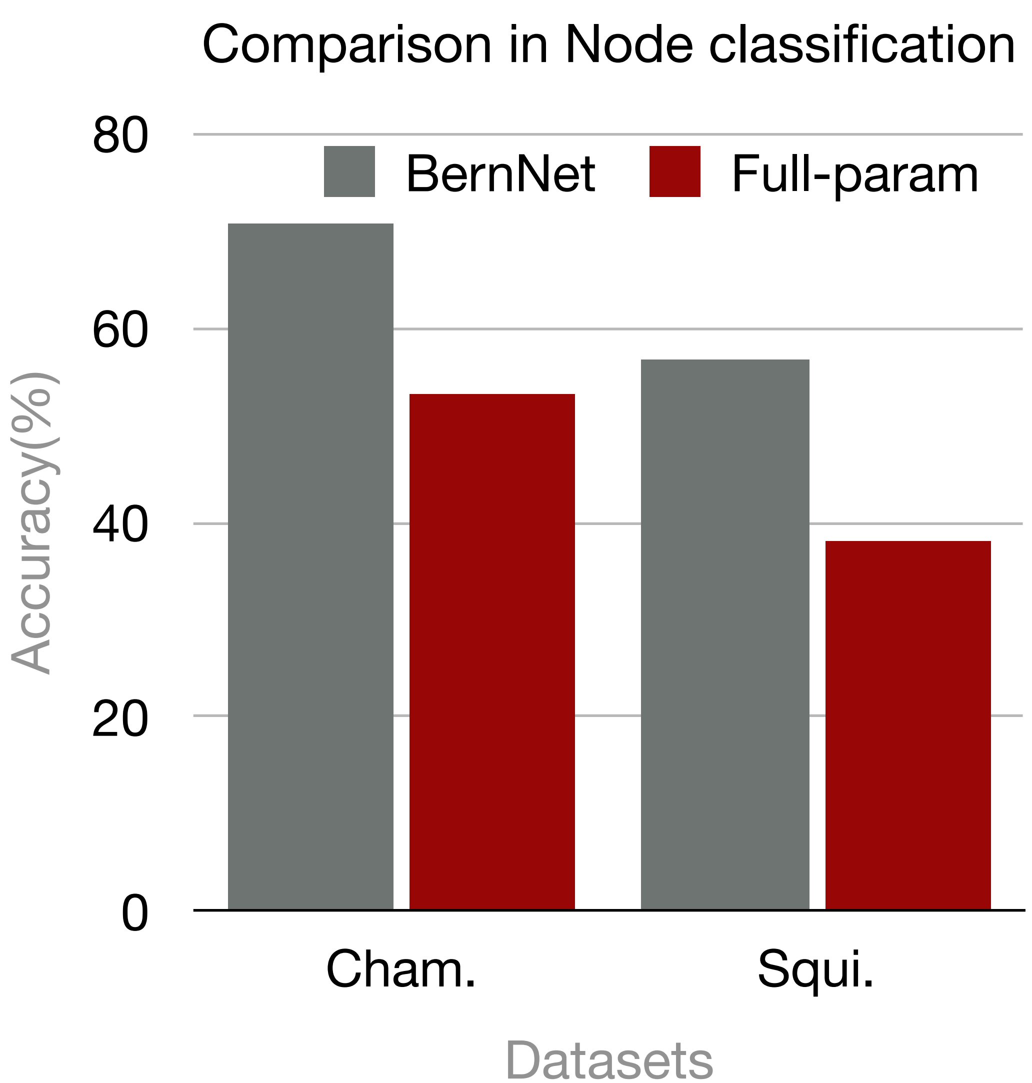
Proposition 1. Suppose a K-order polynomial function $f : [0, 2] \to \mathbb{R}$ with polynomial basis $P_k(\cdot)$ and coefficients $\{\alpha_k\}_{k=0}^{K}$ in real number. For any pair of variables $x, \hat{x} \in [0, 2]$ satisfying $x = \xi \hat{x}$ where ξ is a constant real number, we always have a function $g : [0, 2] \to \mathbb{R}$ with the same polynomial basis but a different set of coefficients $\{\beta_k\}_{k=0}^{K}$ such that $f(x) = g(\hat{x})$.

It allows $\mathbf{S}'_n(i) = \sum_{k=0}^{K} \boxed{\alpha_k P_k(\lambda_{n,i})} \mathbf{U}_n^T \mathbf{X} = \sum_{k=0}^{K} \boxed{\beta_{k,i} P_k(\lambda_i)} \mathbf{U}_n^T \mathbf{X}$

$$\mathbf{Z} = \sum_{k=0}^{K} \textbf{diag}(\beta_{k,1}, \beta_{k,2}, \cdots, \beta_{k,N}) P_k(\hat{\mathbf{L}}) \mathbf{X}$$

Challenges: Complexity & Noise Overfitting

Issue: Parameterizing a large number of filter weights ($\propto$ # nodes) would increase model complexity and cause severe overfitting to local noises.



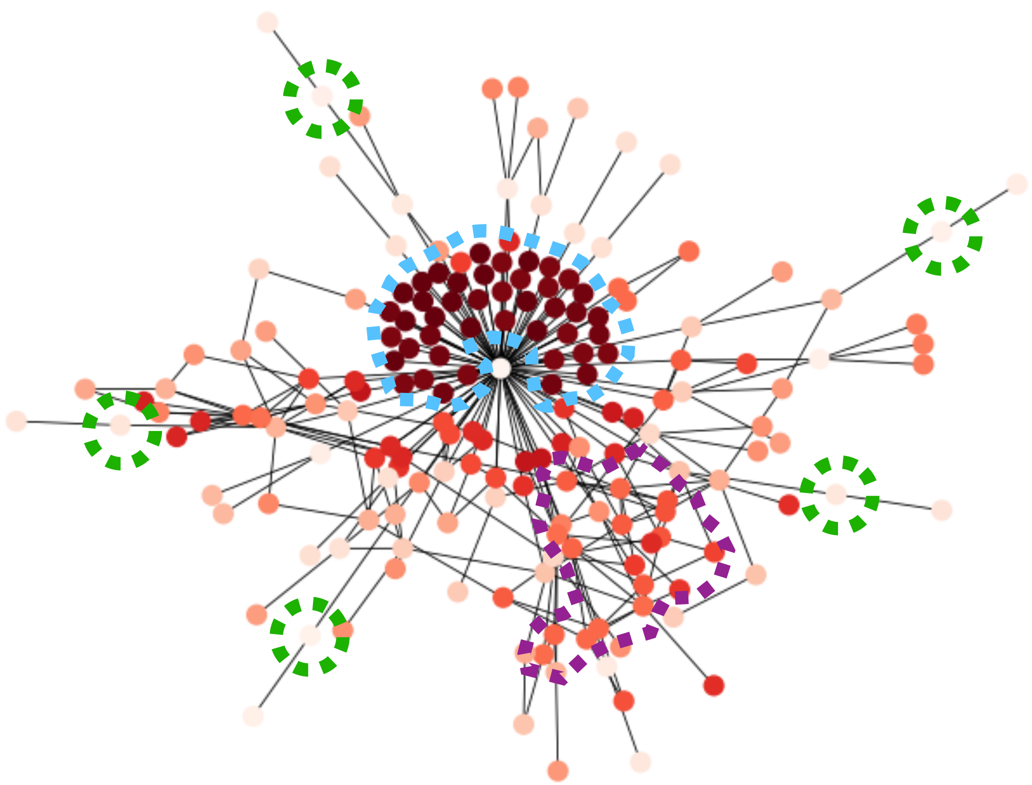
Learning with full-parametrization leads a clear accuracy drop.

"A reason design should be built upon a shared global model whilst locally adapted to each node with awareness of its graph position."

Challenges: Complexity & Noise Overfitting

Observ. 1: Nearby nodes display similar local structures due to their overlapped neighborhoods.

Observ. 2: Distant nodes may still posses alike local context because of the invariant global properties.



Cornell (webpage network): similar color means akin local structure

- Observ. 1 → ■ ■
- Observ. 2 → ■ in •−•−•

DSF: LGWD & Positional-aware Filter Weights

Local and Global Weight Decomposition (LGWD)

global invariant graph properties

$$\beta_{k,i} \leftarrow \gamma_i \cdot \theta_{k,i}$$

local diverse node contexts

Position-aware Filter Weights

$$\arg\min_{\mathbf{P}} \mathscr{L}_P = \|\mathbf{P}^{(0)} - \mathbf{P}\|_2^2 + \kappa_1 tr(\mathbf{P}^T \hat{\mathbf{L}} \mathbf{P}) + \kappa_2 \|\mathbf{P}^T \mathbf{P} - \mathbf{I}\|_2^2$$

$\mathbf{P}$ denotes node positional embeddings

κ_1 and κ_2 are trade-off coefficients

DSF: LGWD & Positional-aware Filter Weights

Position-aware Filter Weights

Iterative gradient method with stepwise $b = \frac{\eta_1}{2}$:

$$\mathbf{P}^{(k)} = \mathbf{P}^{(k-1)} - b \cdot \frac{\partial \mathcal{L}_p}{\partial \mathbf{P}} \bigg|_{\mathbf{P}=\mathbf{P}^{(k-1)}}$$

$$= \eta_1 \mathbf{P}^{(0)} + \left(1 - \eta_1\right) \left(\left(1 + \eta_2\right) \hat{\mathbf{A}} - \eta_2 \left(\mathbf{P}^{(k-1)} \mathbf{P}^{(k-1)^T} \right) \right) \mathbf{P}^{(k-1)}$$

$\theta_{k,i} = \sigma_p(\mathbf{W}^{(k)} \mathbf{P}_i^{(k)} + \mathbf{b}^{(k)})$ for each node v_i $\qquad k = 1,2,\cdots,K$

η_1 and η_2 are constants made up of κ_1 and κ_2

DSF: Overall Algorithm

Current Design → DSF-x-I:

$$\arg\min_{\mathbf{P}} \mathscr{L}_P = \|\mathbf{P}^{(0)} - \mathbf{P}\|_2^2 + \kappa_1 tr(\mathbf{P}^T \hat{\mathbf{L}} \mathbf{P}) + \kappa_2 \boxed{\|\mathbf{P}^T\mathbf{P} - \mathbf{I}\|_2^2}$$

Complexity Overhead with $\mathcal{O}(N^2)$

$$\mathbf{P}^{(k)} = \eta_1 \mathbf{P}^{(0)} + \left(1 - \eta_1\right)\left(\left(1 + \eta_2\right)\hat{\mathbf{A}} - \eta_2 \boxed{\left(\mathbf{P}^{(k-1)}\mathbf{P}^{(k-1)^T}\right)}\right)\mathbf{P}^{(k-1)}$$

Orthogonal Regularization → DSF-x-R:

$$\mathscr{L}_{Orth} = \|\hat{\mathbf{P}}^{(K)}\hat{\mathbf{P}}^{(K)} - \mathbf{I}\|_2^2 \quad \& \quad \eta_2 = 0$$

$$\hat{\mathbf{P}}^{(K)} \xleftarrow{\text{normalization}} \mathbf{P}^{(K)}$$

$$\mathscr{L} = \mathscr{L}_{task} + \lambda_{orth}\mathscr{L}_{orth}$$

$$\boxed{x \in \{\text{GPR}^{[1]}, \text{Bern}^{[2]}, \text{Jacobi}^{[3]}\}}$$

[1] Chien et al. Adaptive Universal Generalized Pagerank Graph Neural Network. In ICLR 2021.
[2] He et al. BernNet: Learning Arbitrary Graph Spectral Filters via Bernstein Approximation. In NeurIPS 2021.
[3] Wang & Zhang. How Powerful are Spectral Graph Neural Networks. In ICML 2022.

DSF: Overall Algorithm

Current Design → DSF-x-I:

Table 1: Average running time per epoch (ms)/average total running time (s). Although DSF-GPR-I is less efficient on large networks, DSF-GPR-R, (our major model) can reduce it by more than 75% on average (though reasonably slower than GPR-GNN).

Datasets	Small-scale	Large-scale	Average
GPR-GNN	1.10/2.24	0.98/5.01	1.08/2.74
DSF-GPR-I	5.96/12.19	40.34/131.77	12.21/33.93
DSF-GPR-R	2.49/6.29	3.02/14.48	2.59/7.78

$$\mathscr{L} = \mathscr{L}_{task} + \lambda_{orth}\mathscr{L}_{orth}$$

$x \in \{\text{GPR}^{[1]}, \text{Bern}^{[2]}, \text{Jacobi}^{[3]}\}$

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[3] Wang & Zhang. How Powerful are Spectral Graph Neural Networks. In ICML 2022.

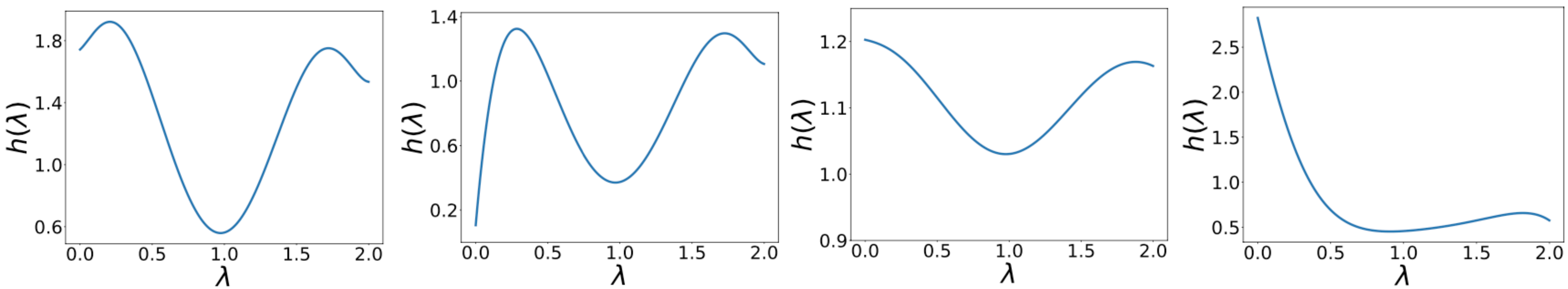
DSF effectively improves SOTAs spectral GNNs

Table 2: Node classification accuracies (%) ± 95% confidence interval over 100 runs. The row of PA-GNN [49]* lists the relative improvements of PA-GNN upon GPR-GNN based on the results obtained from its paper, where – denotes values not provided. Our Improv. gives the best relative improvements between our DSF variants over their common underlying model.

Datasets	Heterophilic Graphs						Homophilic Graphs				
	Chameleon	Squirrel	Wisconsin	Cornell	Texas	Twitch-DE	Cora	Citeseer	Pubmed	Computers	Photo
GCN [24]	67.22±0.43	54.21±0.41	59.45±0.72	52.76±1.17	61.66±0.71	73.94±0.15	88.13±0.25	77.00±0.27	89.07±0.11	91.06±0.12	93.99±0.12
GAT [40]	67.72±0.41	52.26±0.58	57.94±0.89	50.20±0.93	55.37±1.10	73.00±0.15	88.47±0.22	77.23±0.27	88.30±0.11	91.69±0.11	94.55±0.11
ChebNet [11]	64.85±0.44	48.14±0.33	80.93±0.72	77.98±1.00	75.83±1.20	73.73±0.14	87.64±0.21	76.93±0.24	89.91±0.11	91.65±0.12	95.27±0.07
APPNP [15]	53.66±0.33	36.08±0.36	81.23±0.64	81.29±0.78	79.42±1.05	72.65±0.11	88.70±0.21	77.77±0.24	89.93±0.09	91.62±0.10	94.92±0.09
GNN-LF [51]	54.29±0.36	36.87±0.33	59.85±0.60	62.90±0.98	61.88±0.95	73.03±0.13	88.90±0.25	77.35±0.29	88.89±0.10	91.12±0.11	95.13±0.08
GNN-HF [51]	55.22±0.42	35.45±0.30	68.17±0.72	72.98±1.02	66.66±1.34	71.92±0.13	89.01±0.19	77.74±0.23	89.53±0.10	90.73±0.10	95.26±0.09
FAGCN [6]	68.38±0.51	50.08±0.60	82.11±0.85	79.00±0.93	81.00±0.95	74.15±0.13	88.82±0.20	77.65±0.29	90.13±0.11	91.90±0.11	95.25±0.10
GPR-GNN [9]	69.01±0.50	55.39±0.33	82.72±0.85	80.81±0.78	81.66±1.02	74.07±0.18	89.03±0.20	77.63±0.28	90.10±0.44	92.34±0.13	95.34±0.09
DSF-GPR-I	71.18±0.52	57.08±0.29	**87.64**±0.79	84.76±0.90	85.44±1.05	74.58±0.16	**89.64**±0.20	78.03±0.26	90.26±0.08	92.49±0.12	95.64±0.07
DSF-GPR-R	**71.64**±0.55	**58.44**±0.30	87.43±0.74	**84.93**±0.90	**85.56**±0.93	**74.81**±0.14	89.63±0.17	**78.22**±0.29	**90.51**±0.07	**92.80**±0.12	**95.73**±0.08
Our Improv.	2.63%	3.05%	4.92%	4.12%	3.9%	0.74%	0.61%	0.59%	0.41%	0.46%	0.39%
PA-GNN [49]*	0.66%	1.28%	–	–	–	–	-0.09%	-0.74%	-0.03%	1.03%	0.02%
BernNet [20]	70.59±0.42	56.63±0.32	85.00±0.94	82.10±0.95	82.20±0.98	74.45±0.15	88.72±0.23	77.52±0.29	90.21±0.46	92.57±0.10	95.42±0.08
DSF-Bern-I	72.95±0.53	59.45±0.32	**88.23**±0.81	**85.07**±0.93	**84.59**±1.07	74.96±0.15	89.05±0.22	**78.32**±0.27	90.40±0.10	92.76±0.10	95.73±0.07
DSF-Bern-R	**73.60**±0.53	**59.99**±0.30	88.02±0.91	84.29±0.93	84.42±1.00	**75.00**±0.15	**89.10**±0.22	78.27±0.26	**90.52**±0.10	**92.84**±0.10	**95.79**±0.06
Our Improv.	3.01%	3.36%	3.23%	2.97%	2.39%	0.55%	0.38%	0.80%	0.31%	0.27%	0.37%
JacobiConv [42]	73.71±0.42	57.22±0.24	83.21±0.68	82.34±0.88	82.42±0.90	74.34±0.12	89.24±0.19	77.81±0.29	89.50±0.47	92.26±0.10	95.62±0.06
DSF-Jacobi-I	74.88±0.39	58.26±0.26	85.34±0.74	**84.54**±0.81	83.68±1.12	74.65±0.13	89.54±0.19	78.18±0.26	89.78±0.09	92.38±0.11	**95.76**±0.07
DSF-Jacobi-R	**75.00**±0.38	**59.23**±0.27	**86.13**±0.70	84.39±0.88	**84.46**±0.81	**74.75**±0.15	**89.66**±0.19	**78.23**±0.25	**90.07**±0.10	**92.44**±0.11	95.75±0.08
Our Improv.	1.29%	2.01%	2.92%	2.20%	2.04%	0.41%	0.42%	0.42%	0.41%	0.18%	0.14%

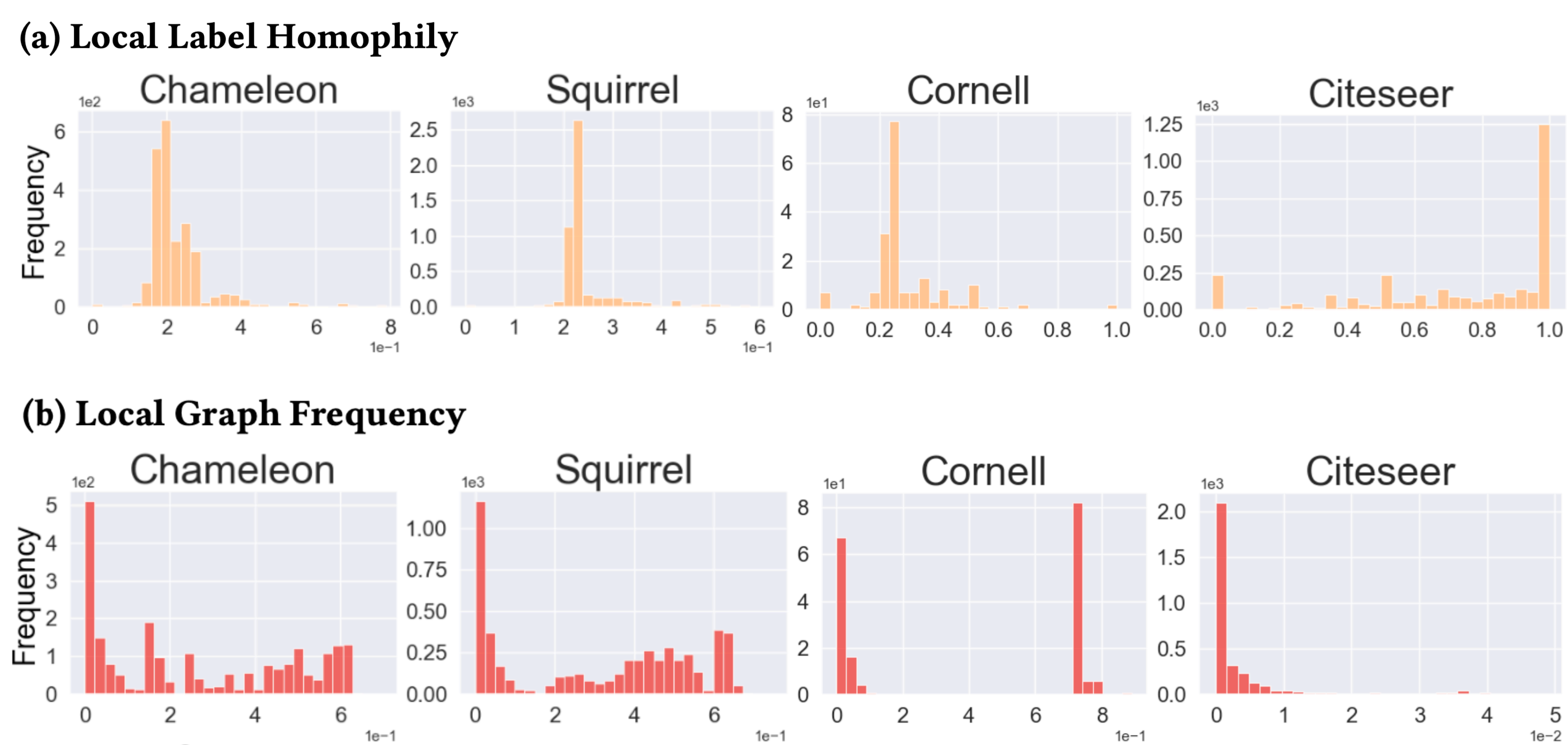
Notable improvement on heterophilic graphs that mostly showcase heterogeneous graph pattern.

Limited interpretability: BernNet learns a single filter



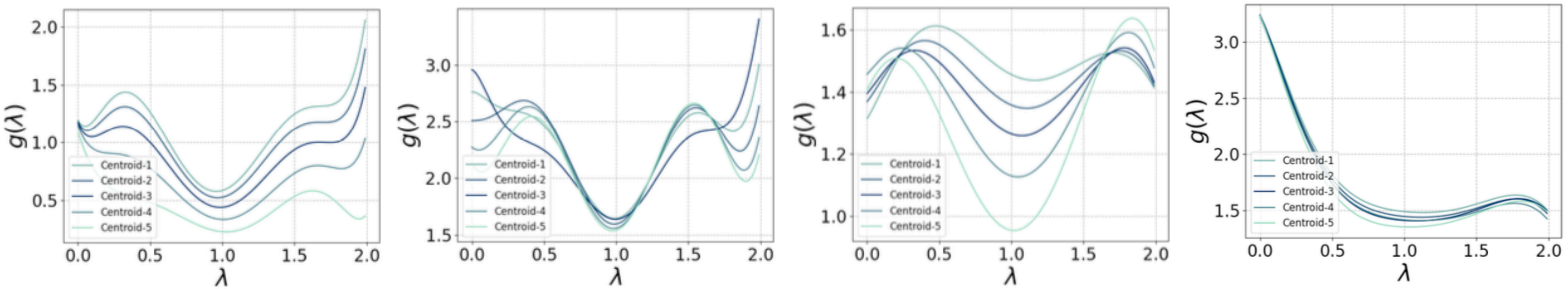
(f) Chameleon (h) Squirrel (j) Cornell (b) CiteSeer

Recall:



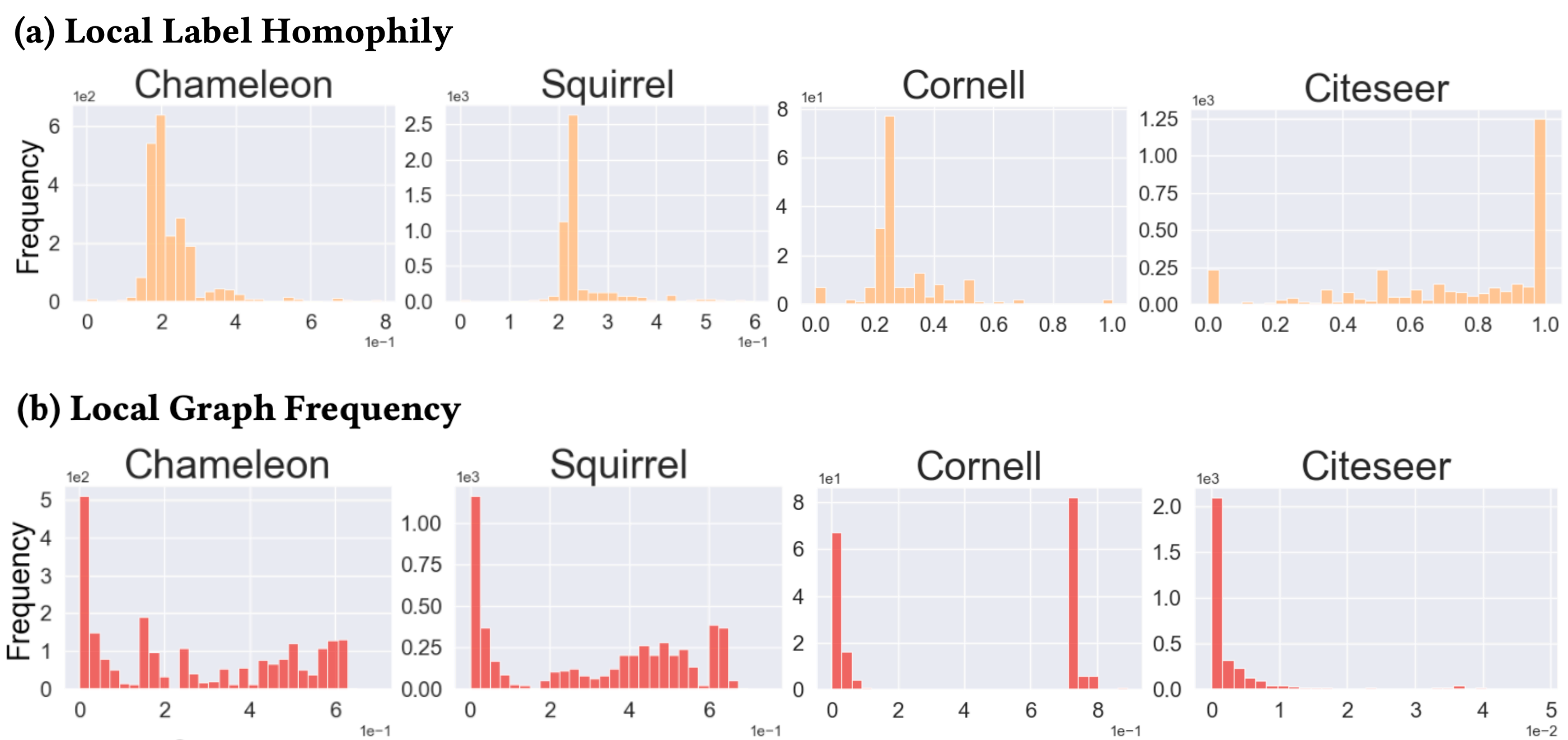
He et al. BernNet: Learning Arbitrary Graph Spectral Filters via Bernstein Approximation. In NeurIPS 2021.

Enhanced Interpretability: DSF learns diverse filters

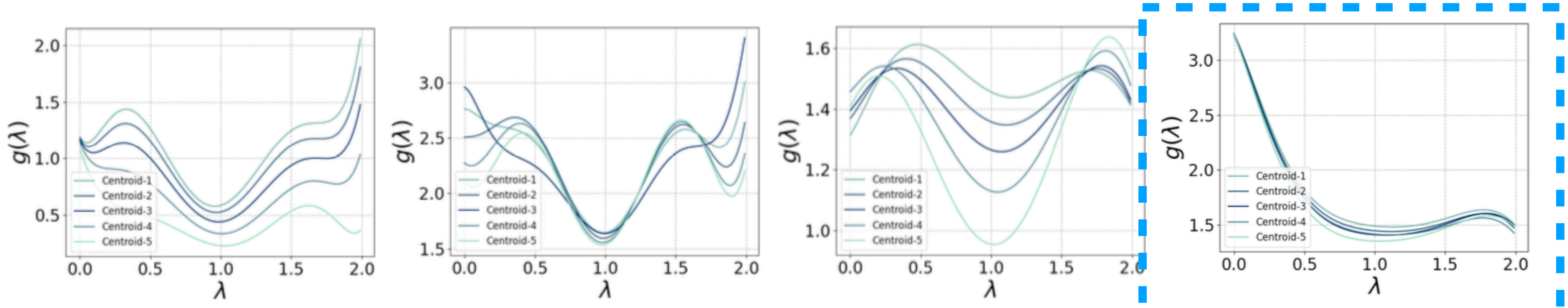


(a) Chameleon **(b) Squirrel** **(c) Cornell** **(d) Citeseer**

Recall:

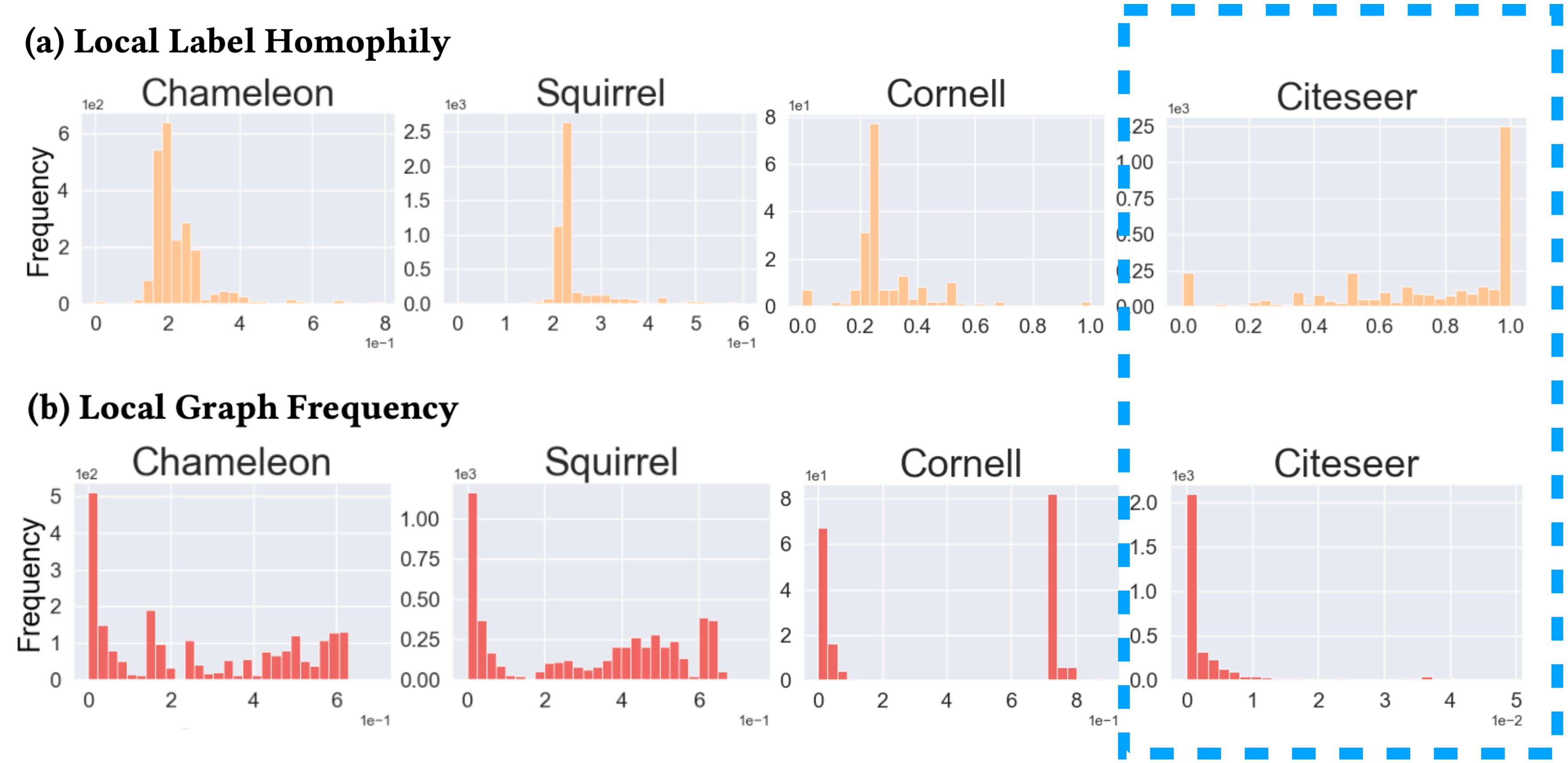


Enhanced Interpretability: DSF learns diverse filters

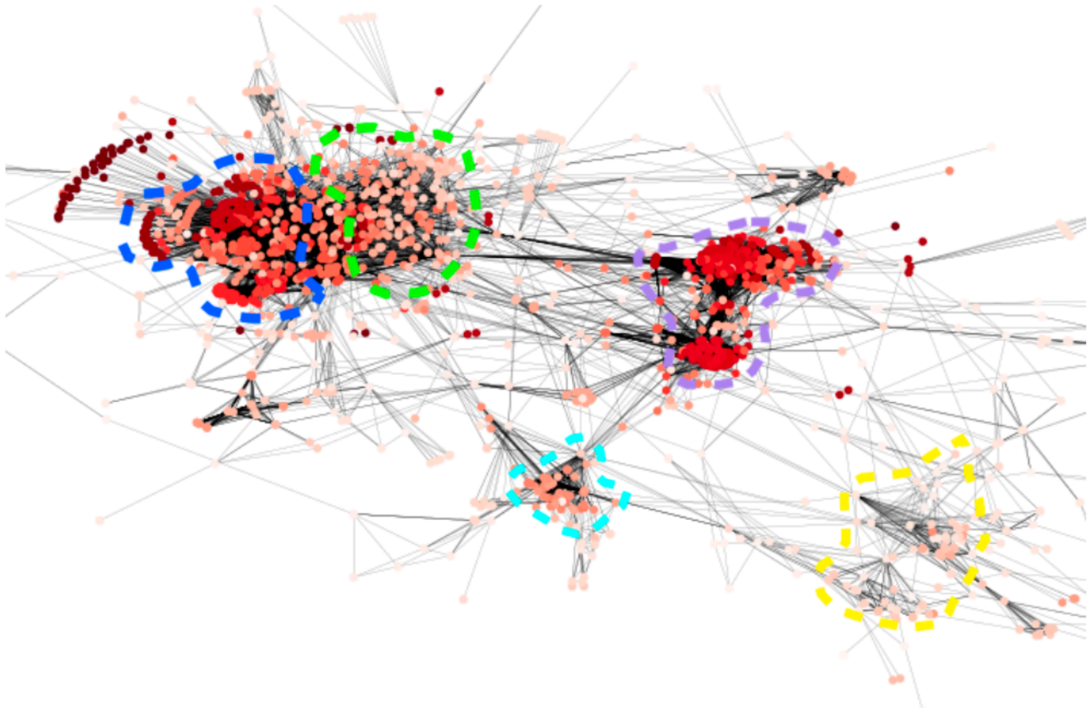


(a) Chameleon (b) Squirrel (c) Cornell (d) Citeseer

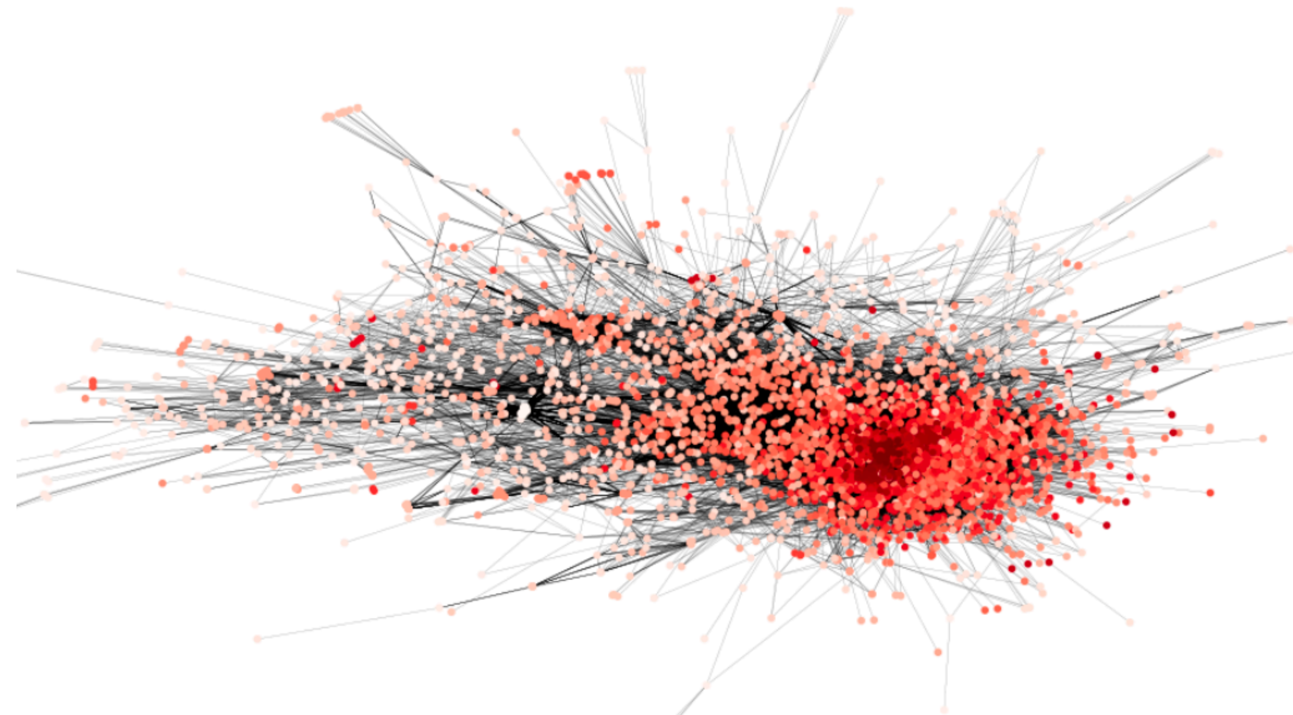
Recall:



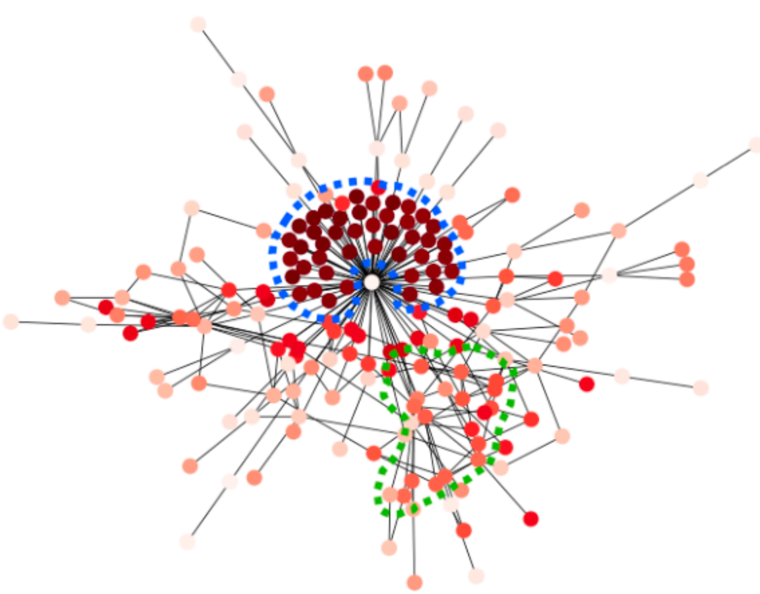
Enhanced Interpretability: DSF learns diverse filters



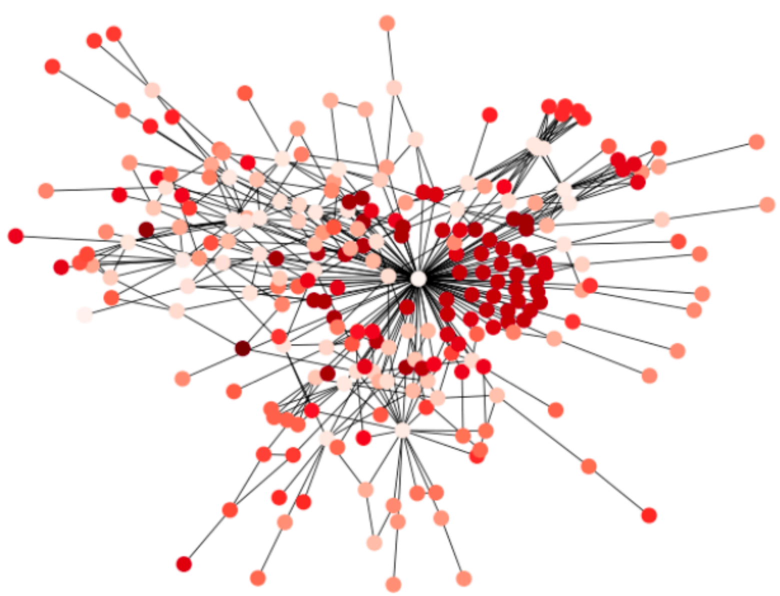
Chameleon



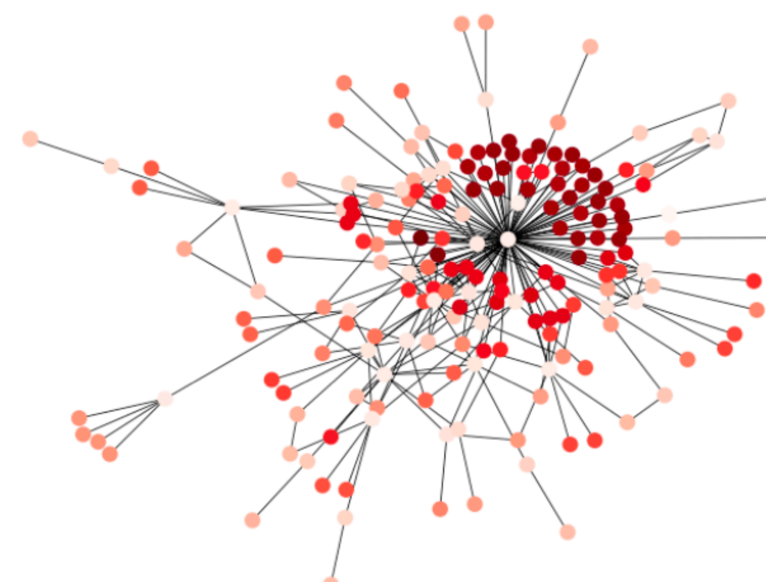
Squirrel



Cornell



Wisconsin



Texas

Our Contributions

- Most spectral GNNs are restricted in a homogeneous spectral filtering.
- Regional heterogeneity is evident in real-world graphs.
- Our DSF learn diverse filters with clear performance gains and enhanced interpretability.

Thank you!

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