Graph Contrastive Learning with Stable and Scalable Spectral Encoding

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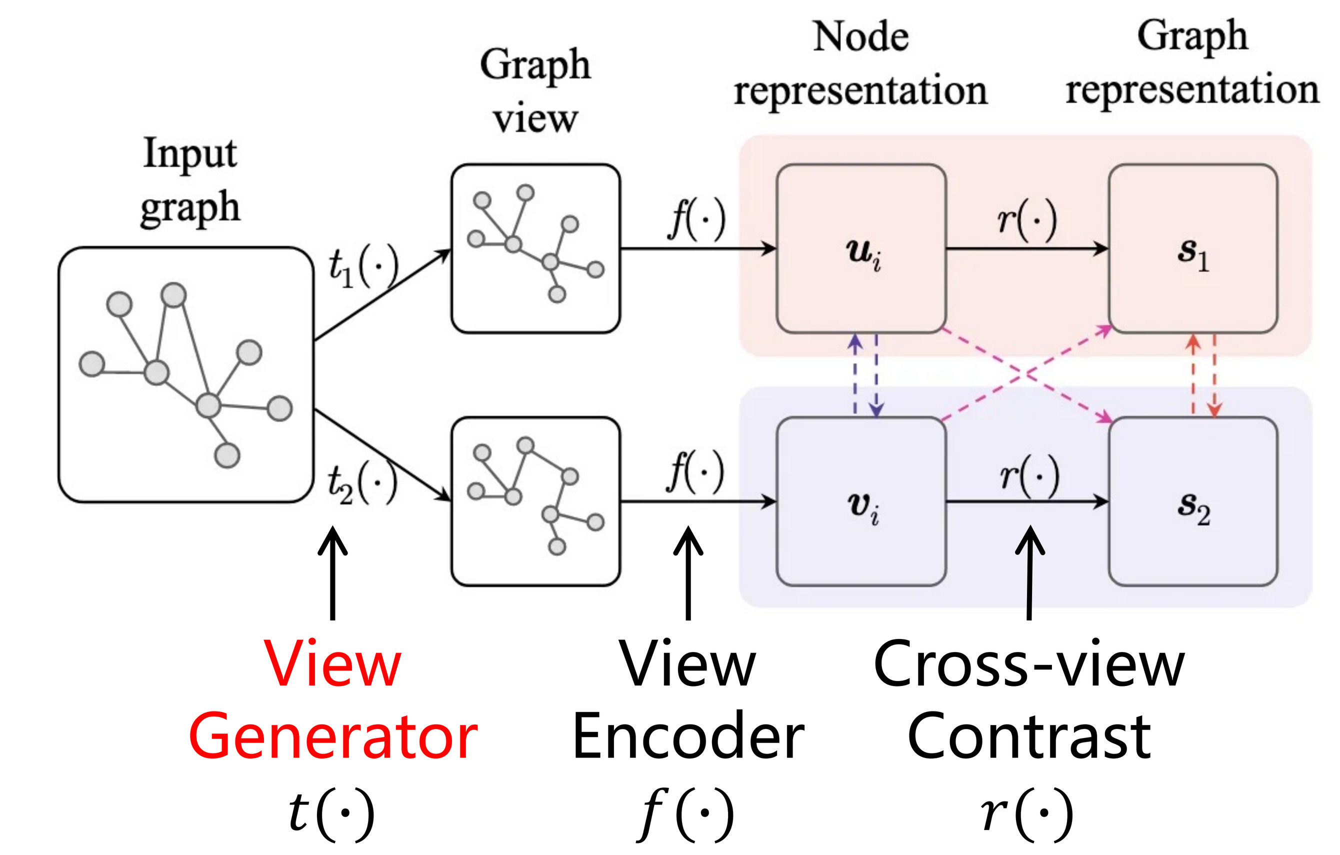
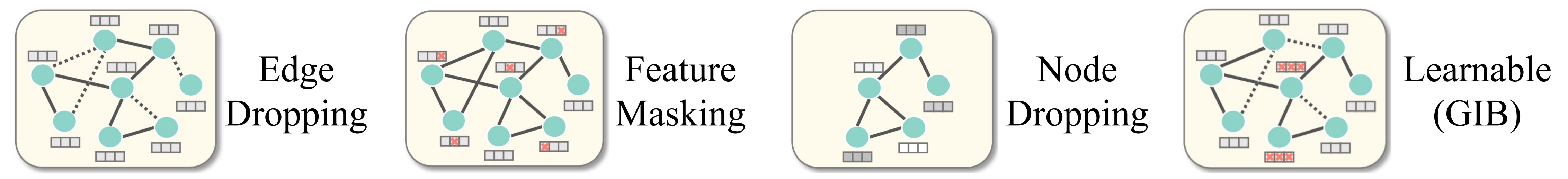
Graph Contrastive Learning



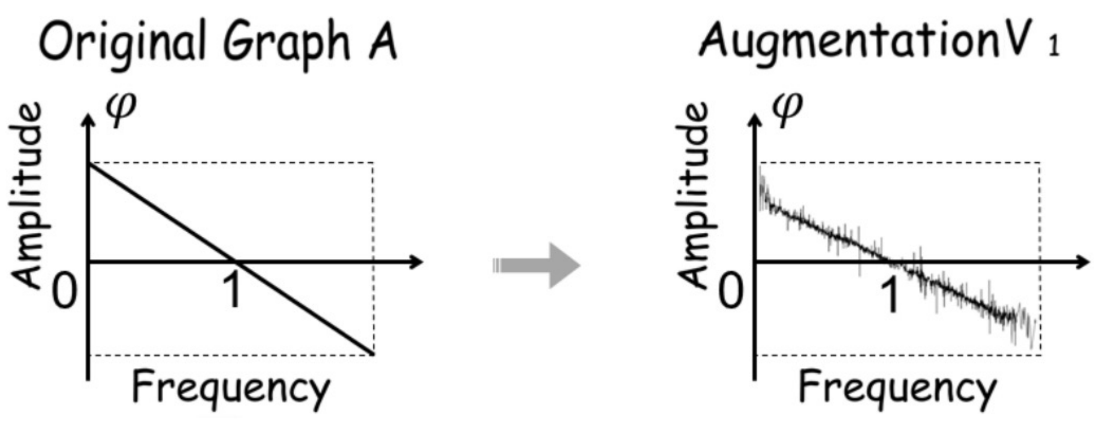
Graph View Generation

➢ Spatial Domain

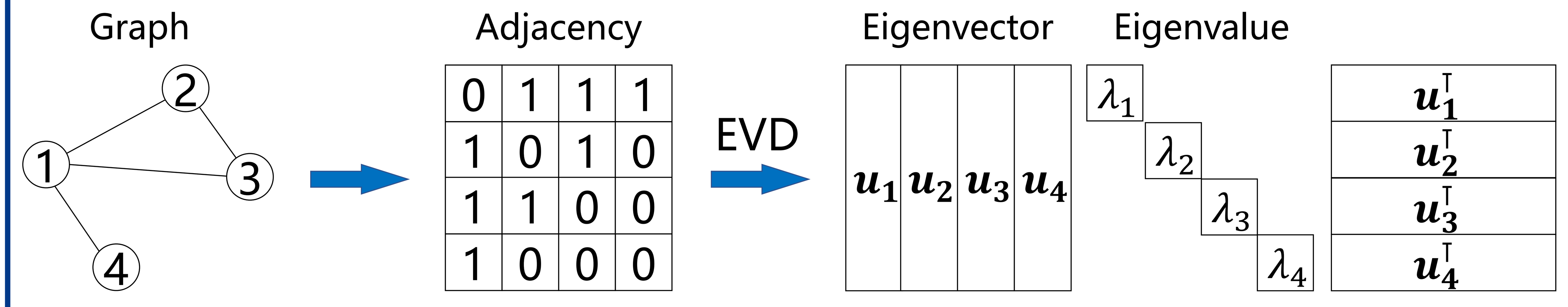


➢ Spectral Domain

- Revisiting Graph Contrastive Learning from the Perspective of Graph Spectrum (NeurIPS 2022)
- Spectral Augmentation for Self-Supervised Learning on Graphs (ICLR 2023)



Spectral View of Graph

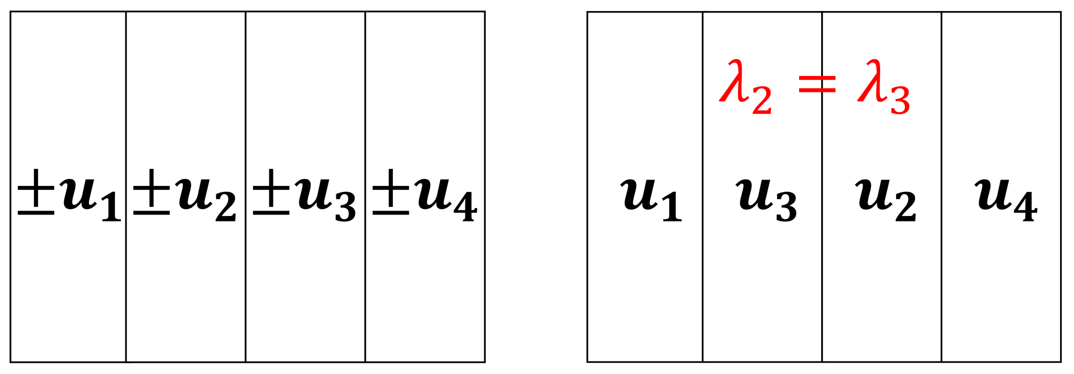


➢Perturb Eigenvalues: $L' = U(\Lambda + \Delta)U^\top$, Complexity: $\mathcal{O}(N^2)\sim\mathcal{O}(N^3)$

➢Perturb Eigenvectors : $L = U\Lambda U^\top = (U\sqrt{\Lambda})(U\sqrt{\Lambda})^\top$, Complexity: $\mathcal{O}(N)$

Pitfall of Eigenvectors

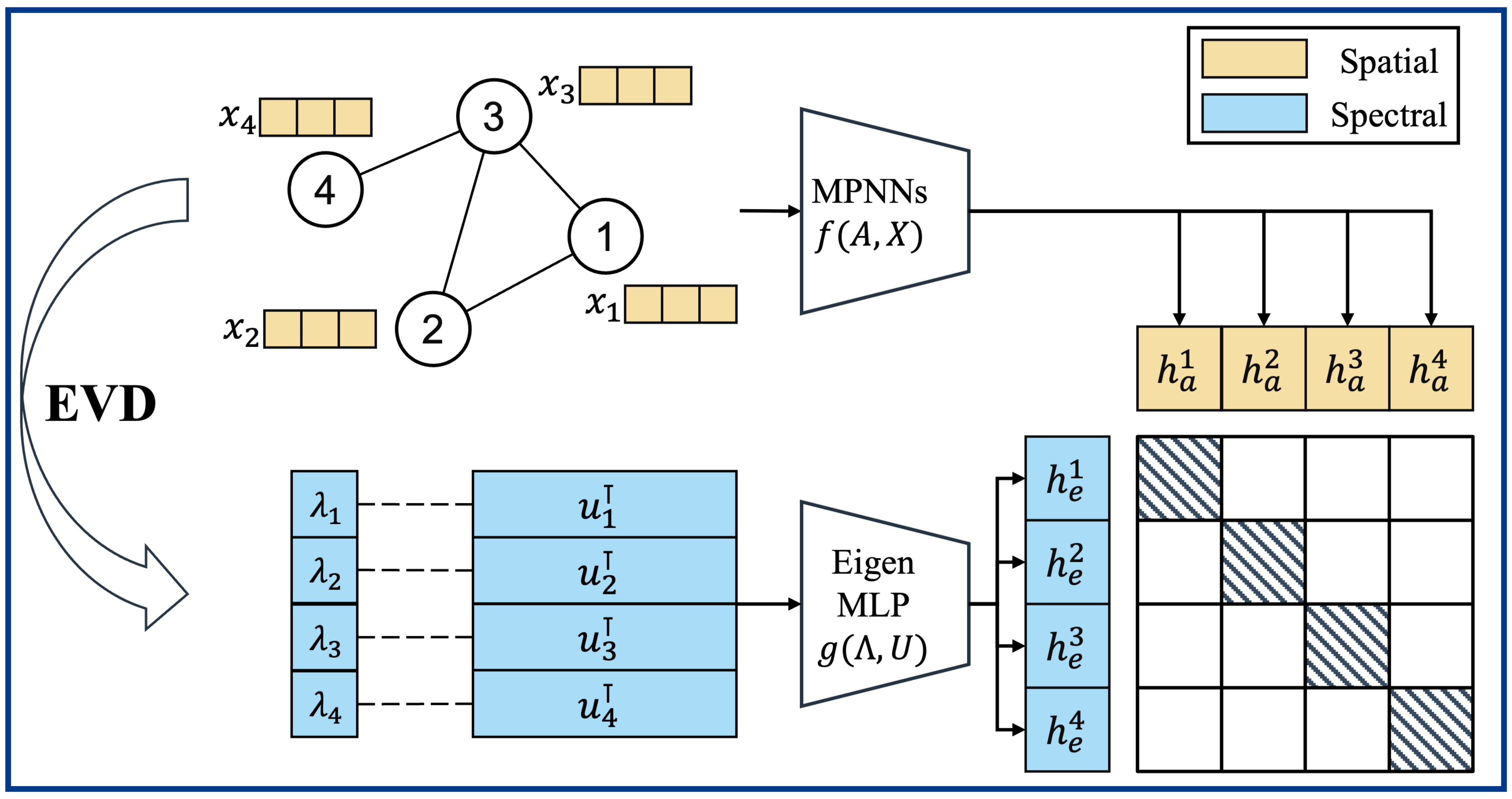
➢Sign-ambiguity ➢Basis-ambiguity



$\boldsymbol{L}\boldsymbol{u}_i = \lambda_i \boldsymbol{u}_i$ $\qquad$ $\boldsymbol{L}\boldsymbol{u}_i = \lambda_i \boldsymbol{u}_i$

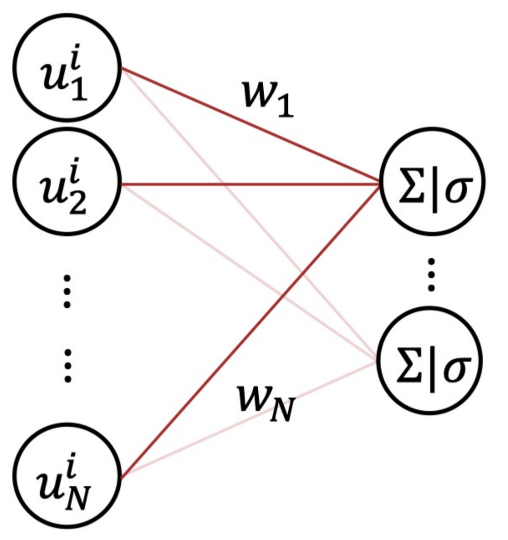
$\boldsymbol{u}_i^\top \boldsymbol{L}\boldsymbol{u}_i = (\pm\boldsymbol{u}_i^\top)\boldsymbol{L}(\pm\boldsymbol{u}_i)$ $\qquad$ $\boldsymbol{L}\boldsymbol{u}_i = \lambda_j \boldsymbol{u}_i$

Method: Sp2GCL & EigenMLP



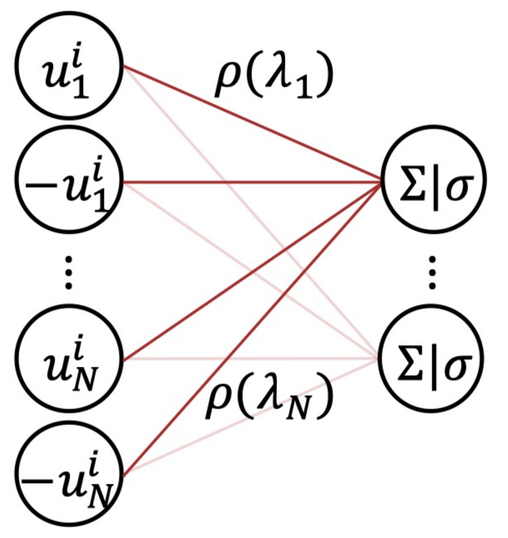
➢Multilayer Perceptron (MLP)

- Efficient and scalable
- Sensitive to input
- $\boldsymbol{H} = \sigma(\boldsymbol{U\Lambda W})$



➢EigenMLP

- Efficient and scalable
- Invariant to the input
- $\boldsymbol{H} = \sigma(\,\varphi(\boldsymbol{U})\,\rho(\boldsymbol{\Lambda})\,\boldsymbol{W})$



Sign- and Basis-invariant

➢Sign-invariant function $\varphi(\boldsymbol{U})$

$$\tilde{\mathbf{U}} = [\psi(\phi(\mathbf{u}_i) + \phi(-\mathbf{u}_i))]_{i=1}^{N}$$

➢Basis-invariant function $\rho(\boldsymbol{\Lambda})$

$$\rho(\lambda) = [\sin(\lambda), \cos(\lambda), \cdots \sin(T\lambda), \cos(T\lambda)]$$

➢Why basis-invariant?

- Eigenvalues are equivariant to the rotation of eigenvectors

$$\underbrace{\begin{bmatrix} u_1^1 & u_2^1 & \cdots & u_k^1 \\ u_1^2 & u_2^2 & \cdots & u_k^2 \\ \vdots & \vdots & \ddots & \vdots \\ u_1^N & u_2^N & \cdots & u_k^N \end{bmatrix}}_{\text{Eigenvectors, } N \times k} \times \underbrace{\begin{bmatrix} \cos(\lambda_1) & \sin(\lambda_1) & \cdots & \cos(T\lambda_1) & \sin(T\lambda_1) \\ \cos(\lambda_2) & \sin(\lambda_2) & \cdots & \cos(T\lambda_2) & \sin(T\lambda_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \cos(\lambda_k) & \sin(\lambda_k) & \cdots & \cos(T\lambda_k) & \sin(T\lambda_k) \end{bmatrix}}_{\text{Fourier features of eigenvalues, } k \times 2T}$$

Experiments

Model	Data	Small Graphs (Full-Batch)			Large Graphs (Mini-Batch)		
		PubMed	Wiki-CS	Facebook	arXiv	Flickr	PPI
GCN	**A**, **X**, **Y**	79.0	77.19±0.12	90.65±0.16	71.74±0.29	49.20±0.31	82.28±0.24
GAT	**A**, **X**, **Y**	79.0±0.3	77.65±0.11	90.47±0.15	71.82±0.23	54.48±0.21	98.85±0.05
DGI	**A**, **X**	76.8±0.6	75.35±0.14	84.42±0.43	70.32±0.25	50.59±0.28	63.80±0.20
BGRL	**A**, **X**	79.6±0.5	79.98±0.13	89.71±0.35	71.54±0.17	51.87±0.15	73.63±0.16
MVGRL	**A**, **X**	80.1±0.7	77.52±0.08	87.29±0.28	-	-	71.45±0.14
GRACE	**A**, **X**	80.6±0.4	80.14±0.48	89.32±0.40	-	-	69.71±0.17
CCA-SSG	**A**, **X**	81.0±0.4	78.85±0.32	89.45±0.60	71.21±0.20	51.66±0.10	73.34±0.17
SpCo	**A**, **X**, **Λ**	81.5±0.4	79.16±0.27	89.98±0.45	-	-	-
SPAN	**A**, **X**, **Λ**	81.5±0.2	**82.13±0.15**	-	-	-	-
Sp^2GCL	**A**, **X**, **Λ**, **U**	**82.3±0.3**	79.42±0.19	**90.43±0.13**	**71.83±0.19**	**52.05±0.33**	**74.28±0.22**

Task	Regression (Metric: RMSE ↓)			Classification (Metric: ROC-AUC% ↑)				
Dataset	molesol	mollipo	molfreesolv	molbace	molbbbp	molclintox	moltox21	molsider
Supervised	1.173±0.057	0.757±0.018	2.755±0.349	72.97±4.00	68.17±1.48	88.14±2.51	74.91±0.51	57.60±1.40
InfoGraph	1.344±0.178	1.005±0.023	10.005±4.819	74.74±3.64	66.33±2.79	64.50±5.32	69.74±0.57	60.54±0.90
GraphCL	1.272±0.089	0.910±0.016	7.679±2.748	74.32±2.70	68.22±1.89	74.92±4.42	72.40±1.01	61.76±1.11
MVGRL	1.433±0.145	0.962±0.036	9.024±1.982	74.20±2.31	67.24±1.39	73.84±4.25	70.48±0.83	61.94±0.94
JOAO	1.285±0.121	0.865±0.032	5.131±0.722	74.43±1.94	67.62±1.29	78.21±4.12	71.83±0.92	62.73±0.92
AD-GCL	**1.217±0.087**	0.842±0.028	5.150±0.624	76.37±2.03	68.24±1.47	<u>80.77±3.92</u>	71.42±0.73	63.19±0.95
SPAN	<u>1.218±0.052</u>	**0.802±0.019**	<u>4.531±0.463</u>	<u>76.74±2.02</u>	**69.59±1.34**	80.28±2.42	<u>72.83±0.62</u>	**64.87±0.88**
Sp^2GCL	1.235±0.119	<u>0.835±0.026</u>	**4.144±0.573**	**78.76±1.43**	<u>68.72±1.53</u>	**80.88±3.86**	**73.06±0.75**	<u>64.23±0.96</u>