SPECTRE:

Spectral Conditioning Helps to Overcome the Expressivity Limits of One-shot Graph Generators

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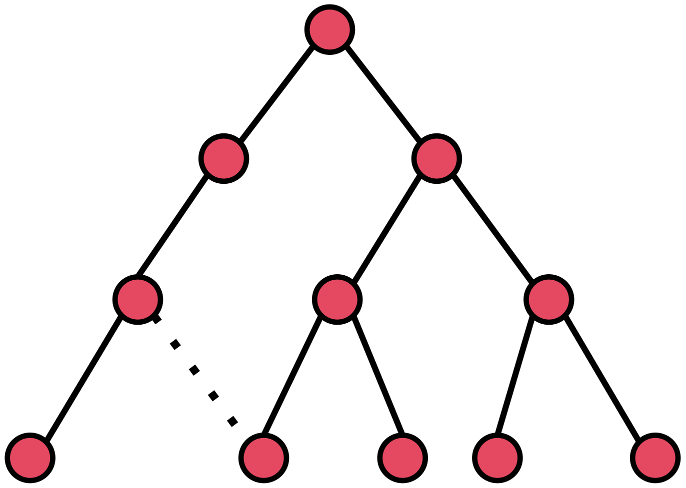
Issues With One-shot Generation

A one-shot generator needs to control the global graph structure by local interactions

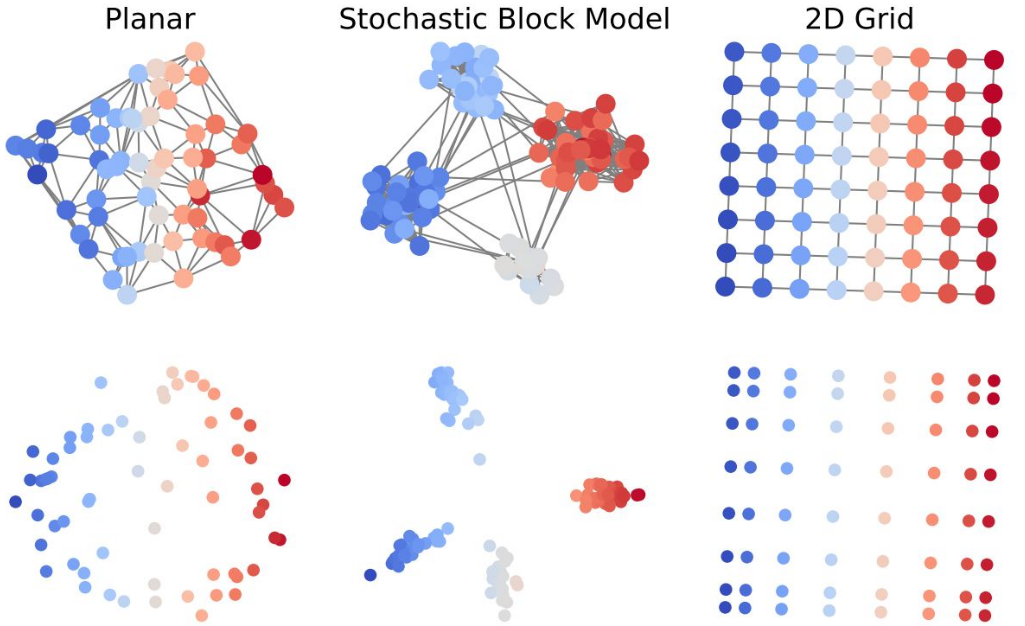
- this becomes harder and harder as the graph becomes larger

Autoregressive methods avoid this adding only a few nodes at a time.



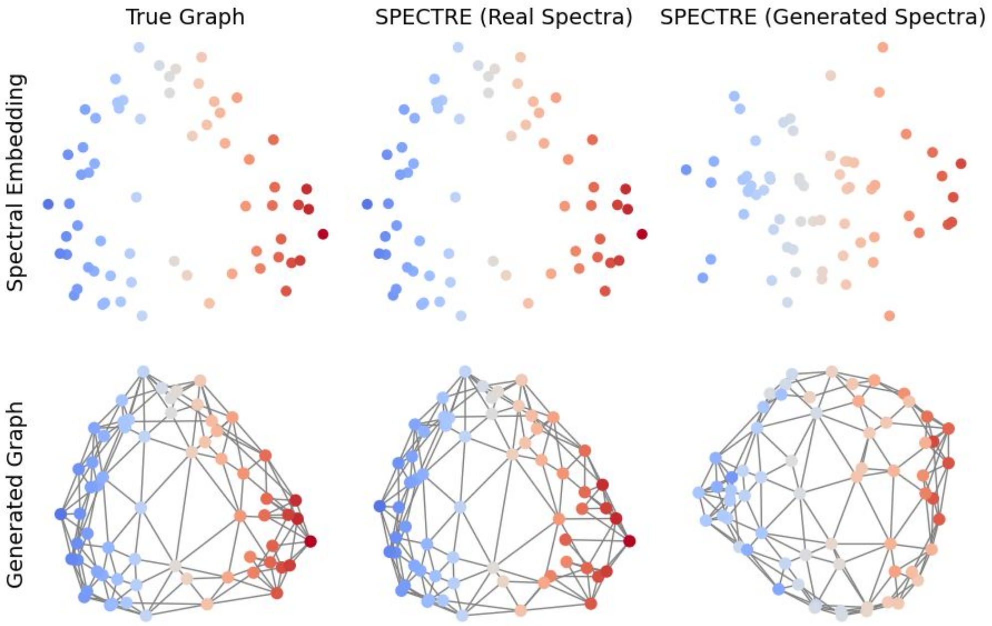
No node can see the cycle without gathering information about the entire graph.

Motivation: Taking Inspiration From Spectral Graph Theory



Idea: generate the top-k eigenvectors/values first and use them to condition the graph generator.

It Works!



True Graph
SPECTRE (Real Spectra)
SPECTRE (Generated Spectra)
Spectral Embedding
Generated Graph

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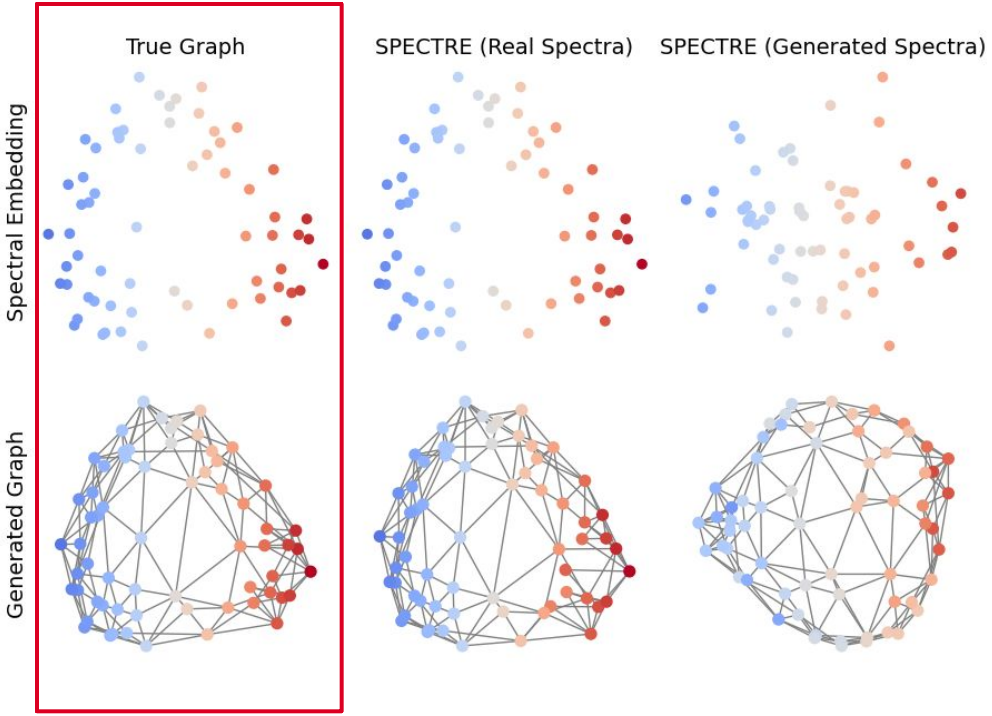
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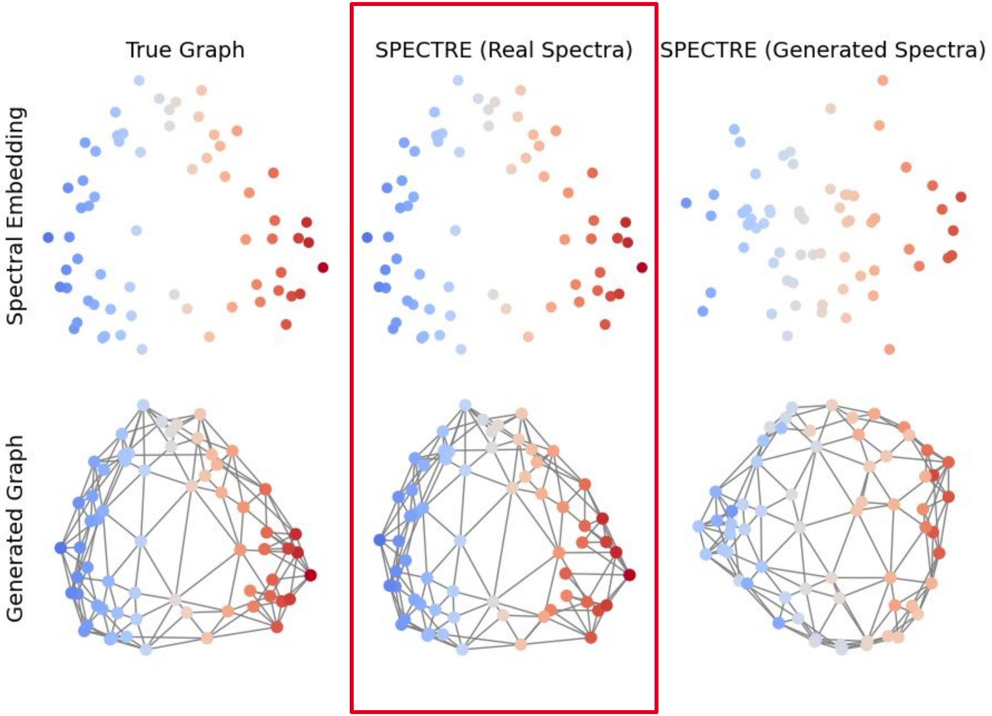
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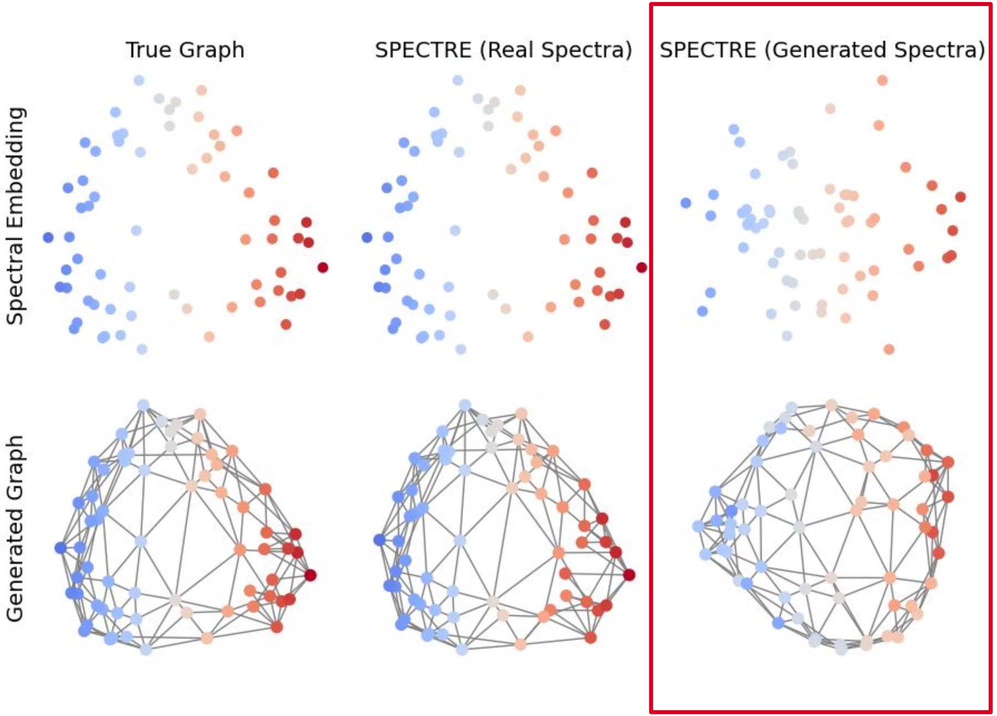
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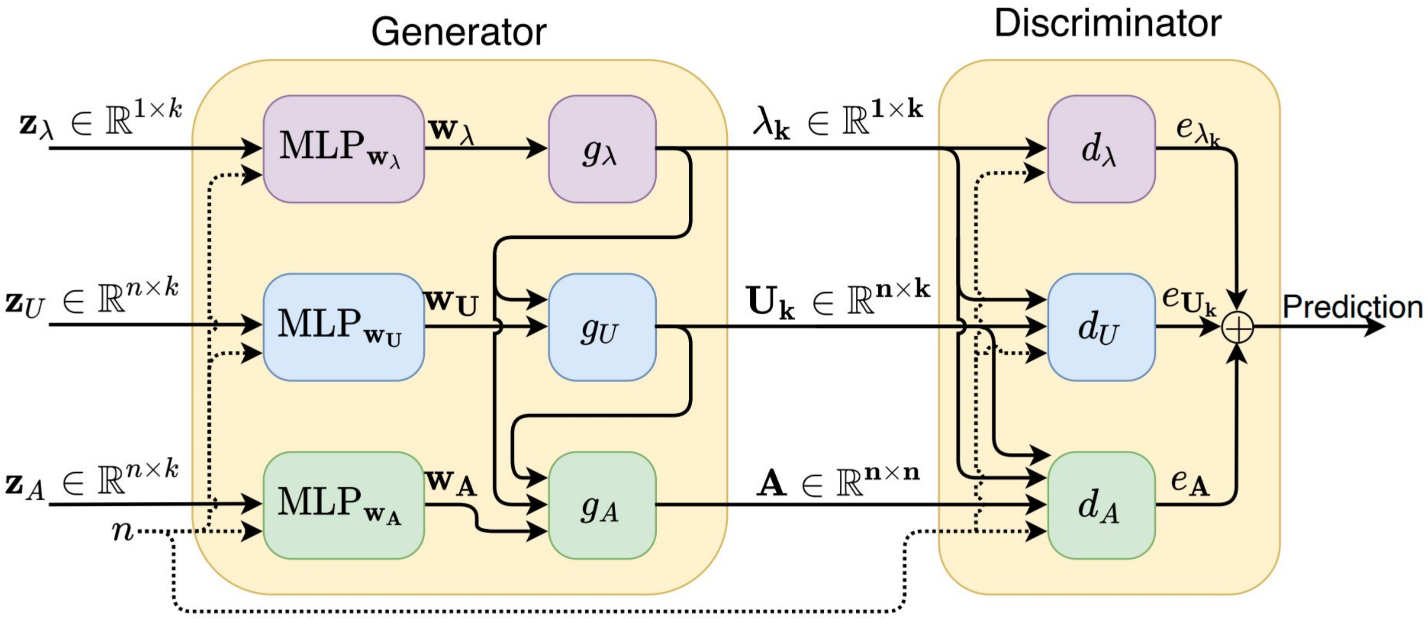
How It Works



Generator
Discriminator
$\mathbf{z}_\lambda \in \mathbb{R}^{1\times k}$
$\mathbf{z}_U \in \mathbb{R}^{n\times k}$
$\mathbf{z}_A \in \mathbb{R}^{n\times k}$
n
$\mathrm{MLP}_{\mathbf{w}_\lambda}$
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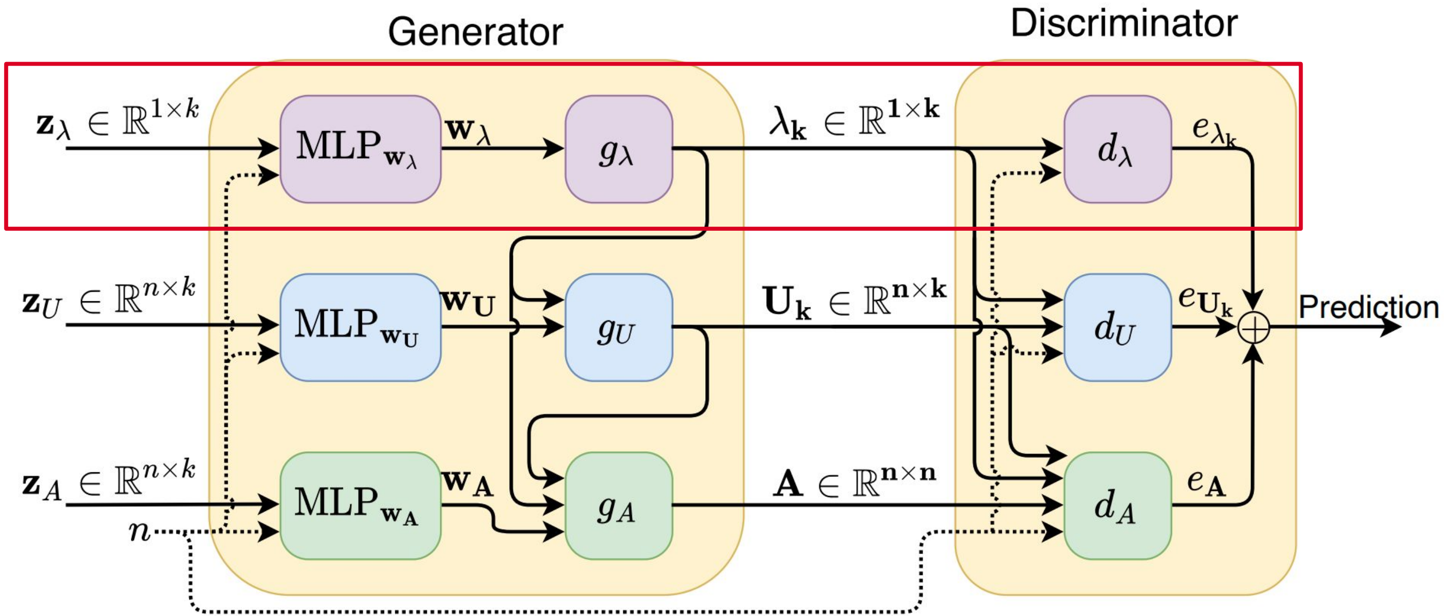

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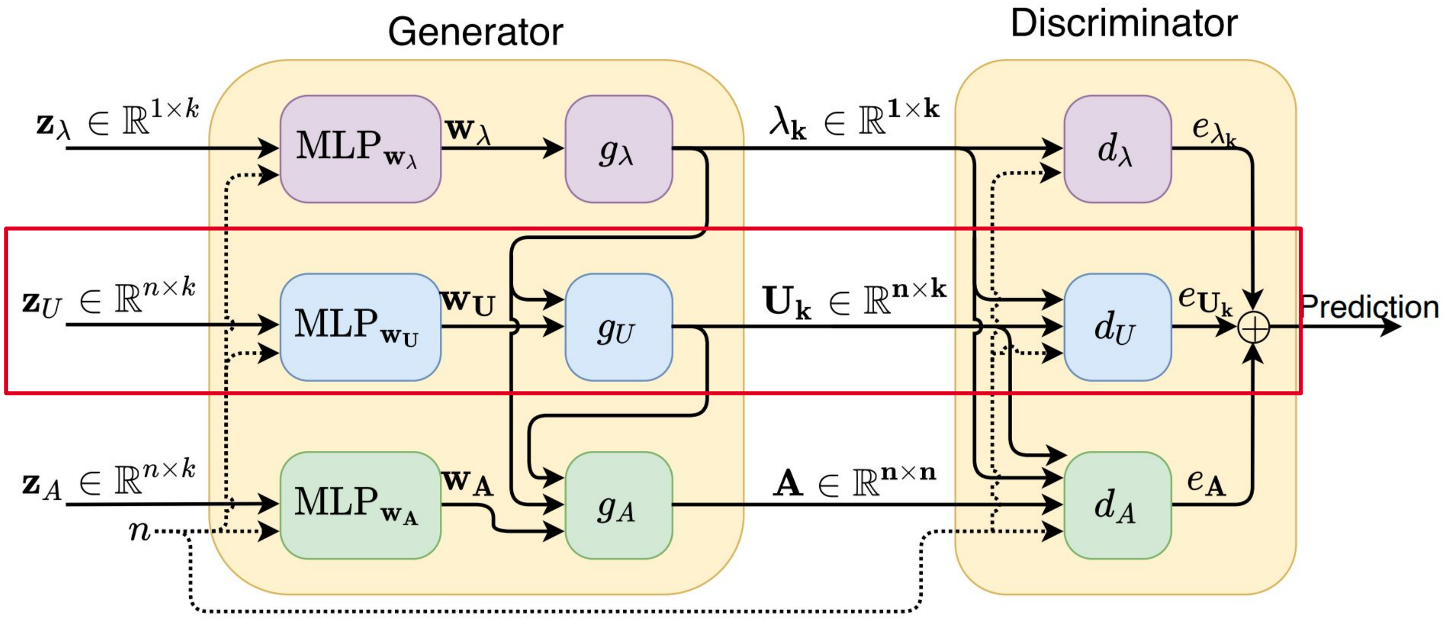

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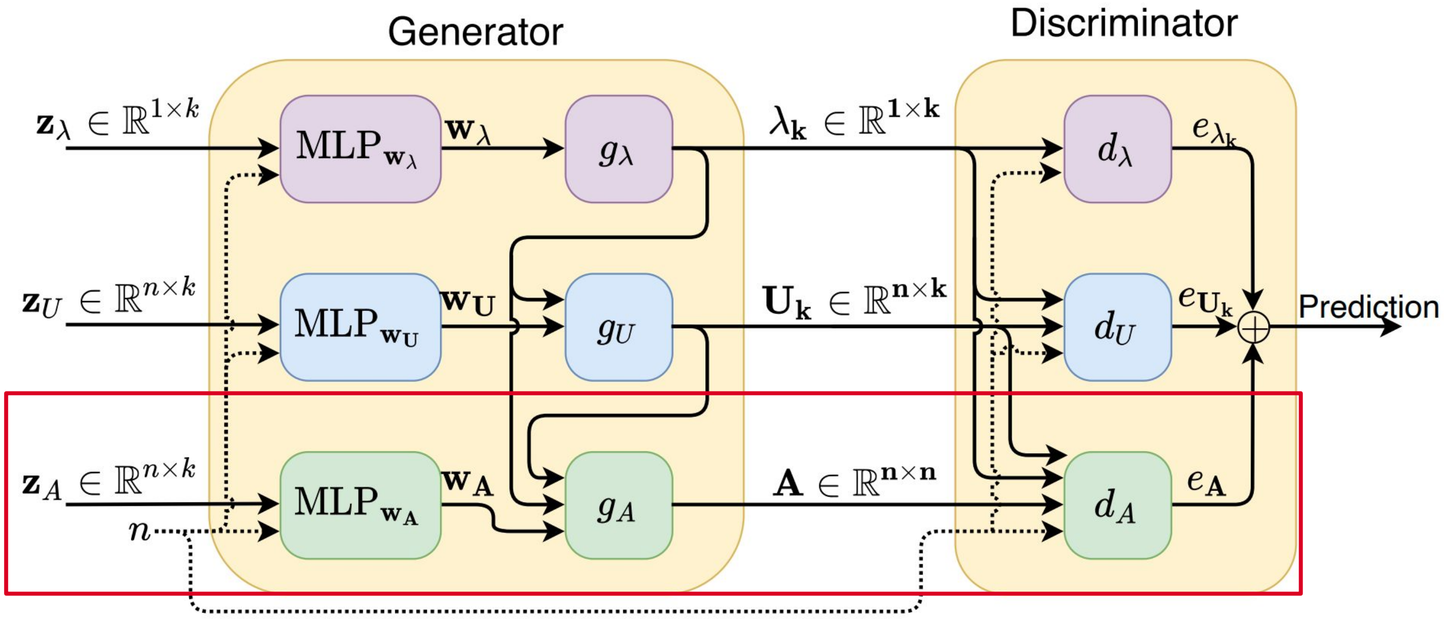

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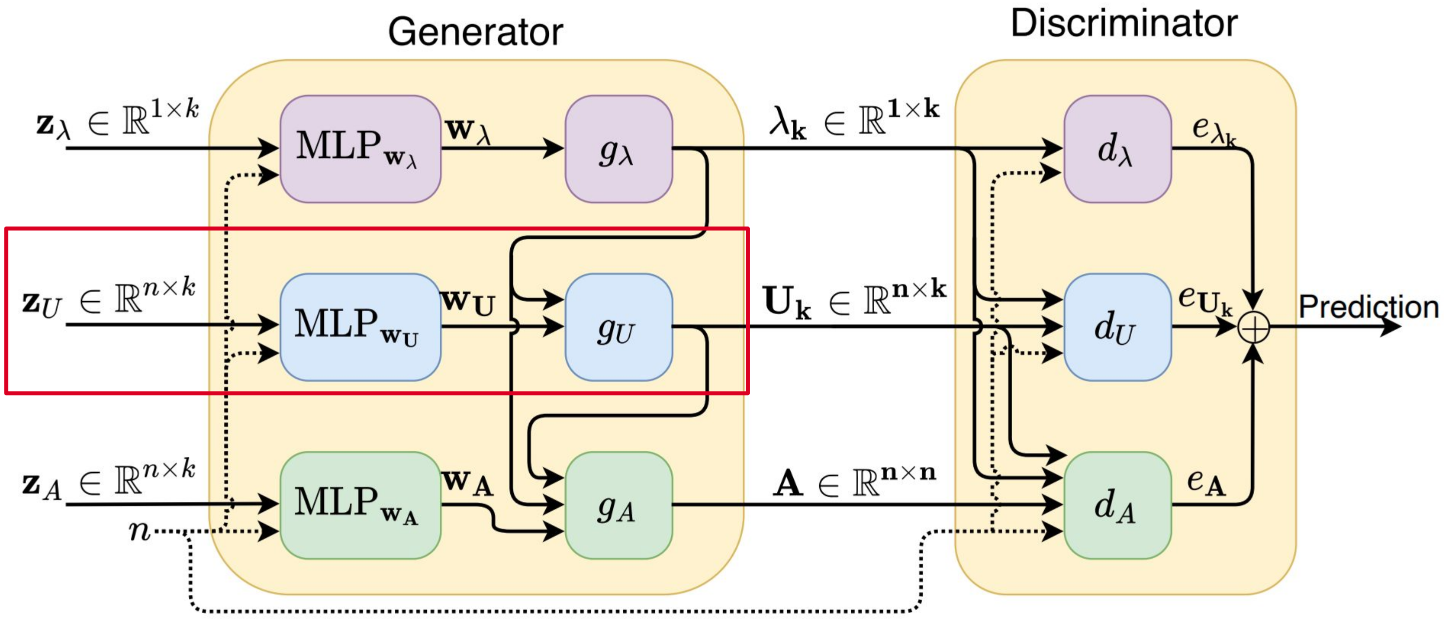

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Eigenvector Refinement

$$\boldsymbol{U}_k^{(\ell)} = \boldsymbol{R}_L^{(\ell)} \boldsymbol{U}_k^{(\ell-1)} \boldsymbol{R}_R^{(\ell)} \quad \text{for layer} \quad \ell = 1, \cdots, L.$$

$$\boldsymbol{U}_k \in \mathbb{R}^{n \times k}$$

$$\boldsymbol{U}_k^\top \boldsymbol{U}_k = \boldsymbol{I}_k$$

$$\boldsymbol{R}_L \in \mathbb{R}^{n \times n}$$

$$\boldsymbol{R}_L^\top \boldsymbol{R}_L = \boldsymbol{I}_n$$

$$\boldsymbol{R}_R \in \mathbb{R}^{k \times k}$$

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Eigenvector Refinement

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$$\boxed{\begin{array}{c} \boldsymbol{U}_k \in \mathbb{R}^{n \times k} \\ \boldsymbol{U}_k^\top \boldsymbol{U}_k = \boldsymbol{I}_k \end{array}}$$

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Eigenvector Refinement

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$$\boxed{\begin{gathered} \boldsymbol{R}_L \in \mathbb{R}^{n \times n} \\ \boldsymbol{R}_L^\top \boldsymbol{R}_L = \boldsymbol{I}_n \end{gathered}}$$

$$\boldsymbol{R}_R \in \mathbb{R}^{k \times k}$$

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Eigenvector Refinement

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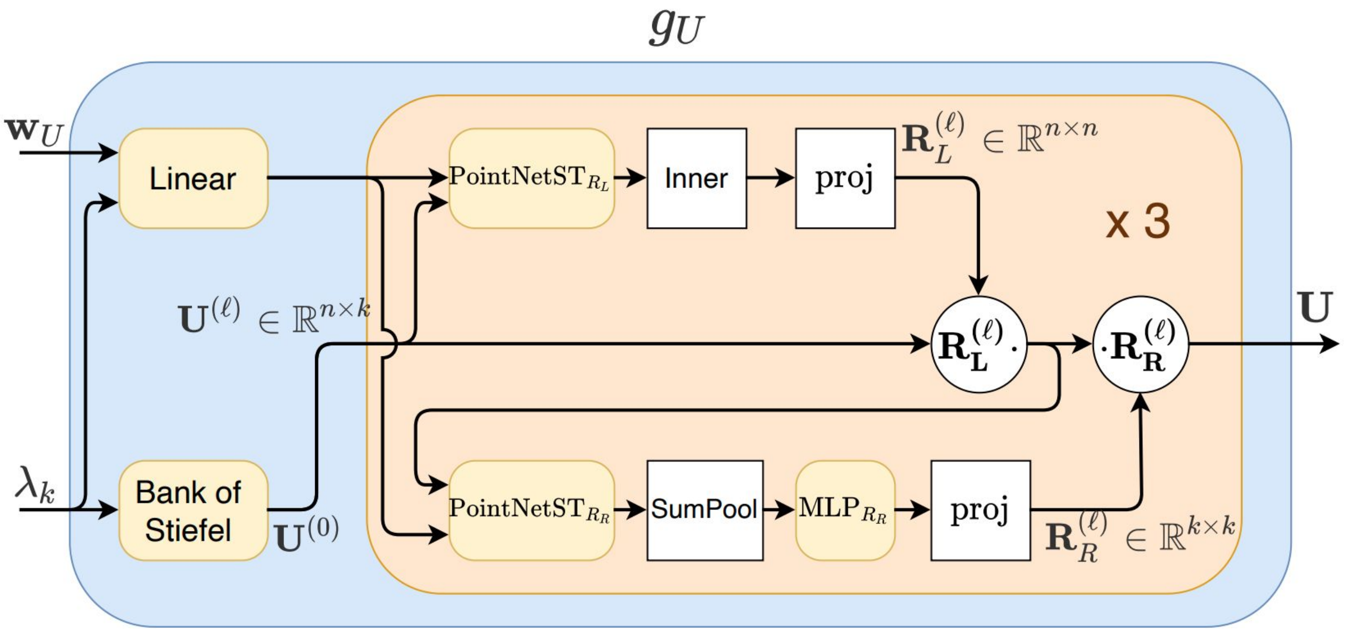
$$\boldsymbol{R}_R \in \mathbb{R}^{k \times k}$$

$$\boldsymbol{R}_R^\top \boldsymbol{R}_R = \boldsymbol{I}_k$$

Eigenvector Generator



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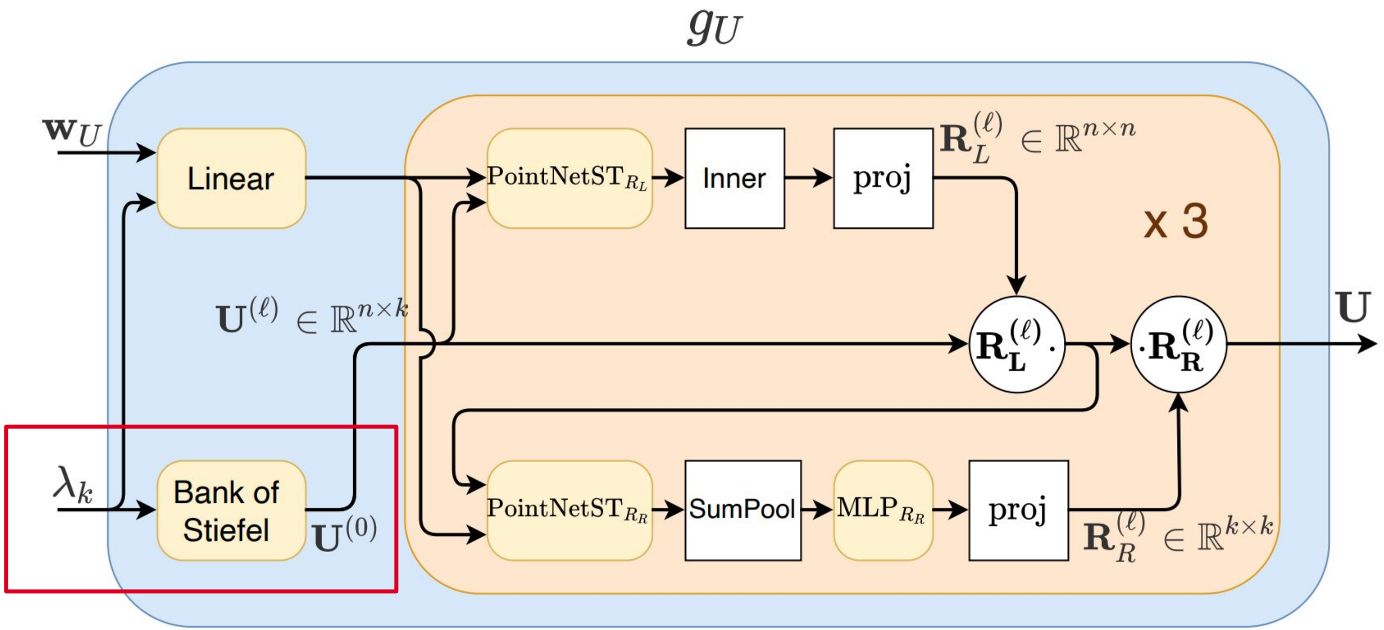

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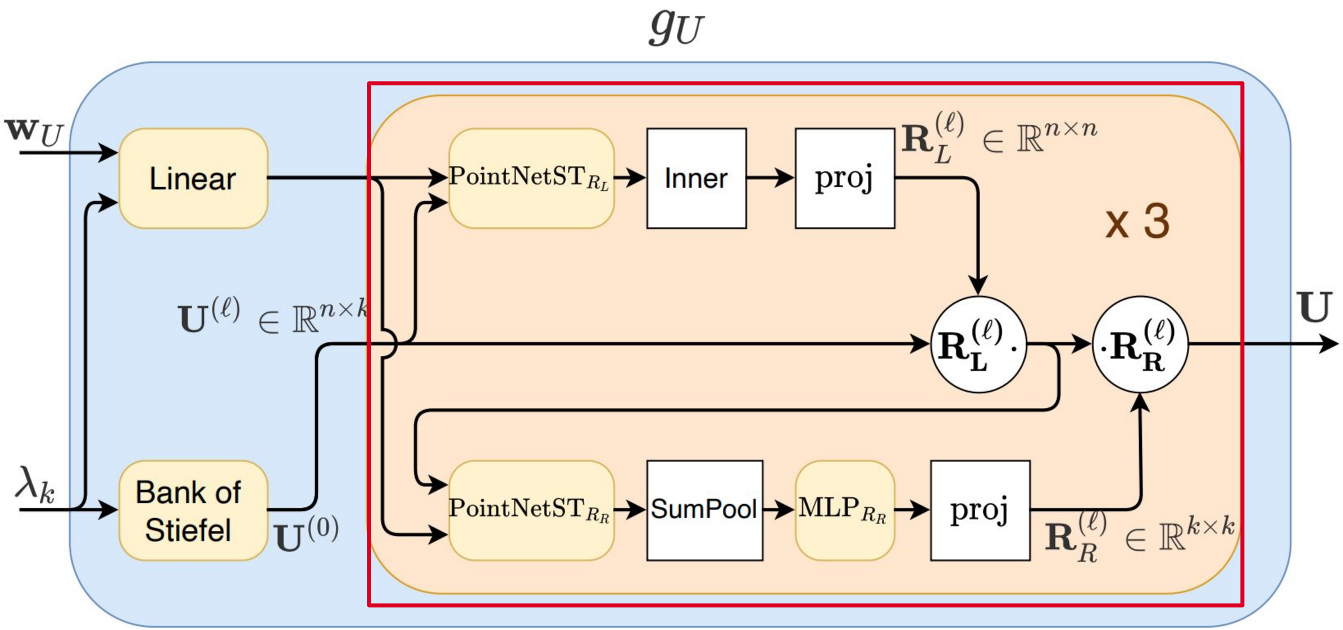

Some Numbers

	Planar graphs										
Model	Deg. ↓	Clus. ↓	Orbit ↓	Spec. ↓	Wavelet ↓	Ratio ↓	Valid ↑	Unique ↑	Novel ↑	Val., Uniq. & Nov. ↑	t (s) ↓
Training set	0.0002	0.0310	0.0005	0.0052	0.0012	1.0	100.0	100.0	—	—	—
GraphRNN	0.0049	0.2779	1.2543	0.0459	0.1034	527.4	0.0	100.0	100.0	0.0	0.774
GRAN	0.0007	0.0426	0.0009	0.0075	0.0019	1.9	97.5	85.0	2.5	0.0	0.920
MolGAN*	0.0009	0.3164	1.1730	0.1989	0.0729	491.9	0.0	25.0	100.0	0.0	0.002
GG-GAN (RS)*	0.1005	0.2571	1.0313	0.2040	0.3829	586.3	0.0	100.0	100.0	0.0	0.011
GG-GAN*	0.0630	1.1820	1.2280	0.1990	0.1890	601.0	0.0	10.0	100.0	0.0	0.011
SPECTRE ($k = 2$)	0.0005	0.0785	0.0012	0.0112	0.0059	2.9	25.0	100.0	100.0	25.0	0.026
SPECTRE ($k = 2$, real spectra)	0.0010	0.0668	0.0010	0.0095	0.0056	3.1	47.5	100.0[‡]	100.0[‡]	47.5[‡]	0.011

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GraphRNN	0.0055	0.0584	0.0785	0.0065	0.0431	14.9	5.0	100.0	100.0	5.0	5.108
GRAN	0.0113	0.0553	0.0540	0.0054	0.0212	9.8	25.0	100.0	100.0	25.0	1.887
MolGAN*	0.0235	0.1161	0.0712	0.0117	0.0292	15.8	10.0	95.0	100.0	9.5	0.002
GG-GAN (RS)*	0.0338	0.0581	0.1019	0.0613	0.1749	61.5	0.0	100.0	100.0	0.0	0.056
GG-GAN*	0.0035	0.0699	0.0587	0.0094	0.0202	7.8	25.0	100.0	100.0	25.0	0.057
SPECTRE ($k = 4$)	0.0015	0.0521	0.0412	0.0056	0.0028	2.0	52.5	100.0	100.0	52.5	0.074
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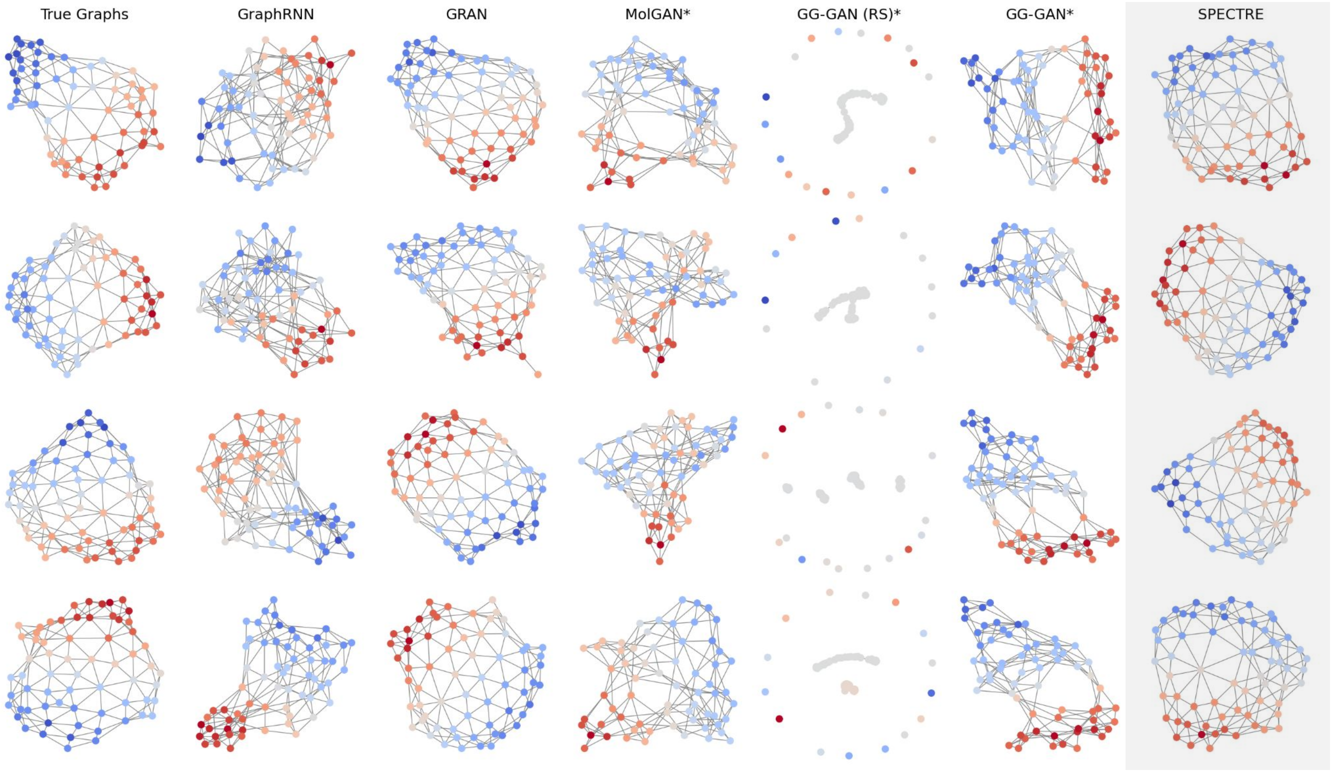
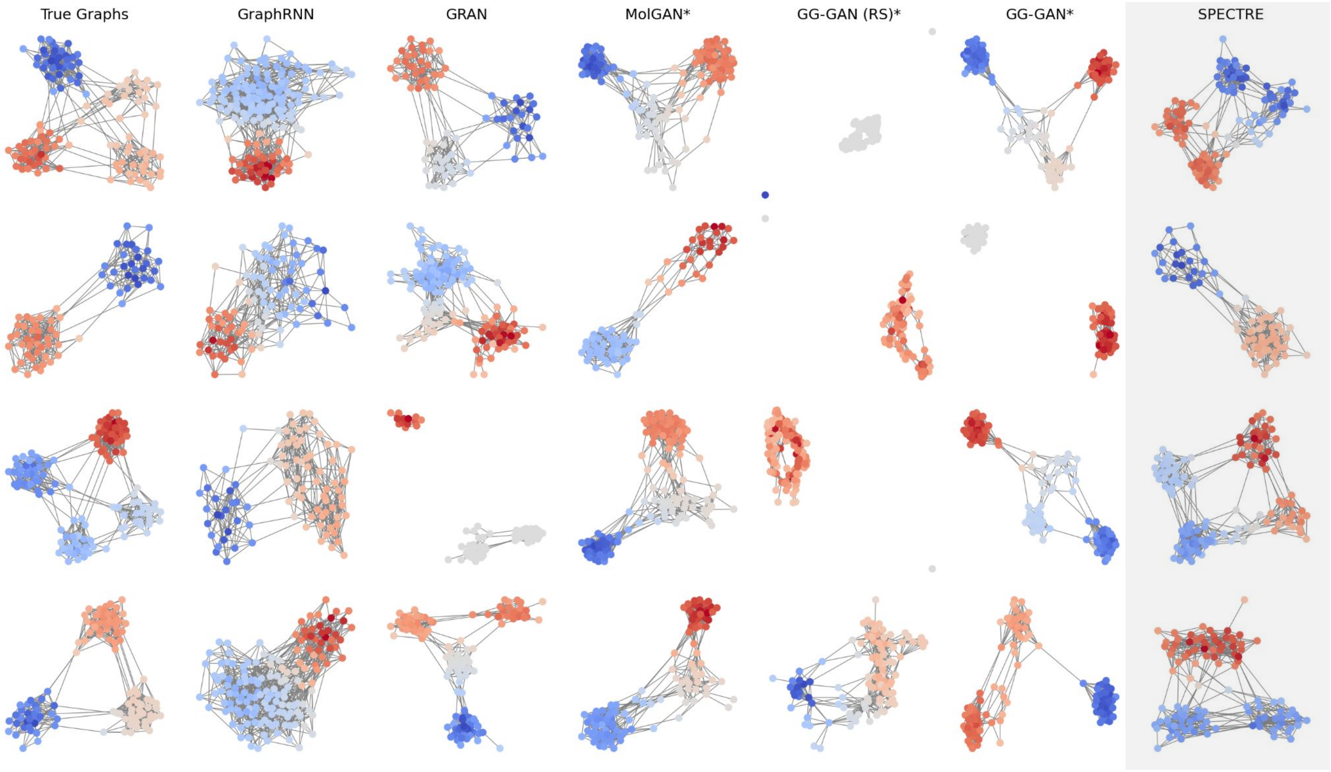
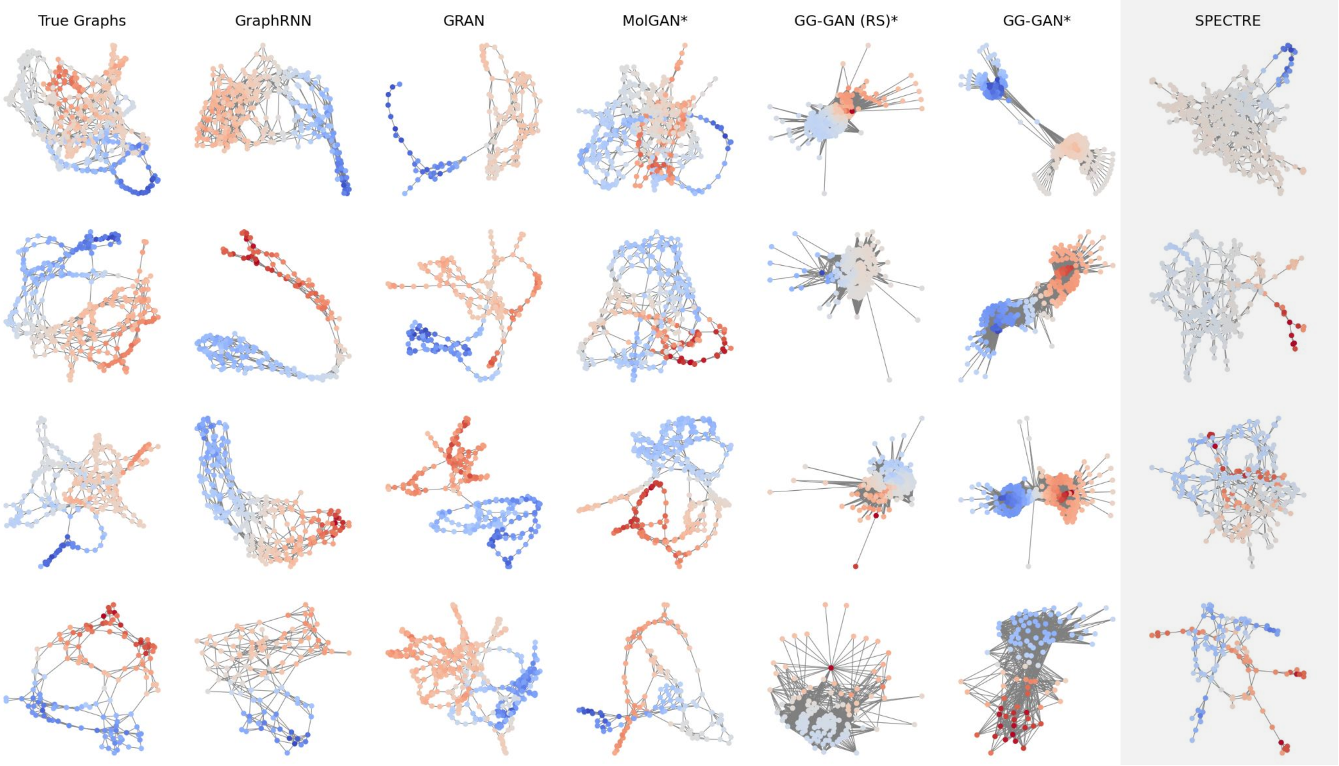


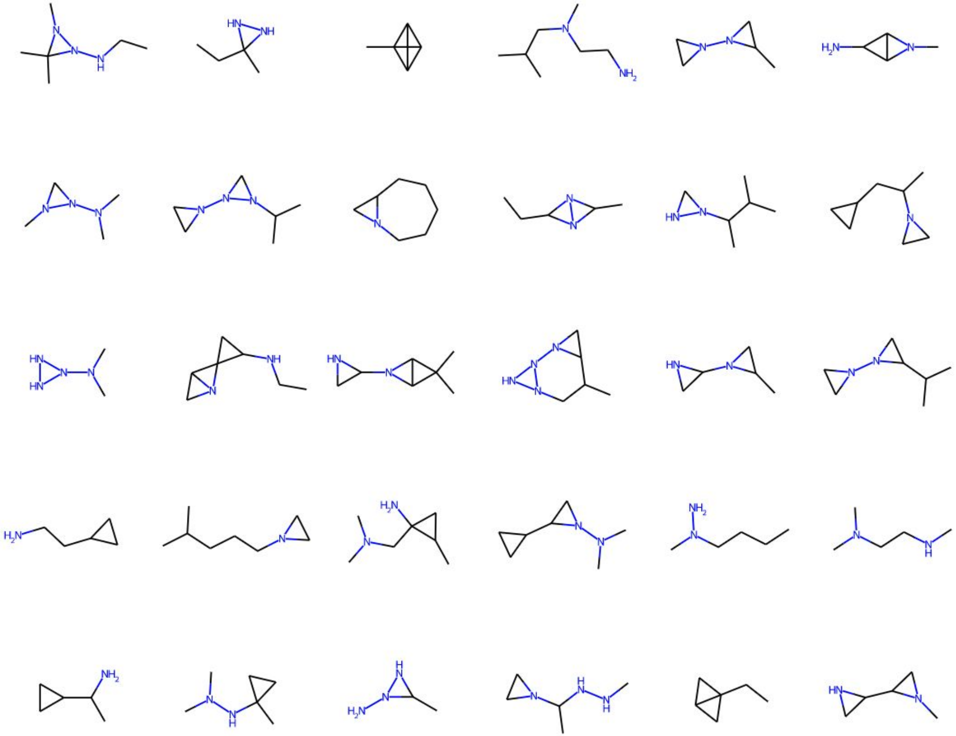
Stochastic Block Model Graphs



Protein Graphs



Molecular Graphs



Limitations - Potential for Future Work!

- Complex architecture
- Large memory requirements (OOM on 24GB GPU for ~600 node graphs)
- Generating eigenvectors is hard

Dataset	Eigenvalue	Wavelet (true)	Wavelet (fake)
Planar (k=2)	17.60	45.43	206.15
SBM (k=4)	9.39	7.01	19.46
Proteins (k=16)	36.83	4.94	23.42

Spectral MMD ratios

Prescient Design

A Genentech Accelerator

is hiring!

https://bit.ly/3wtzENf

twitter.com/prescientdesign

Bibliography

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[2] Jiaxuan, et al. "GraphRNN: Generating realistic graphs with deep auto-regressive models." ICML 2018.

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