AdaSpec: Adaptive Spectrum for Enhanced Node Distinguishability

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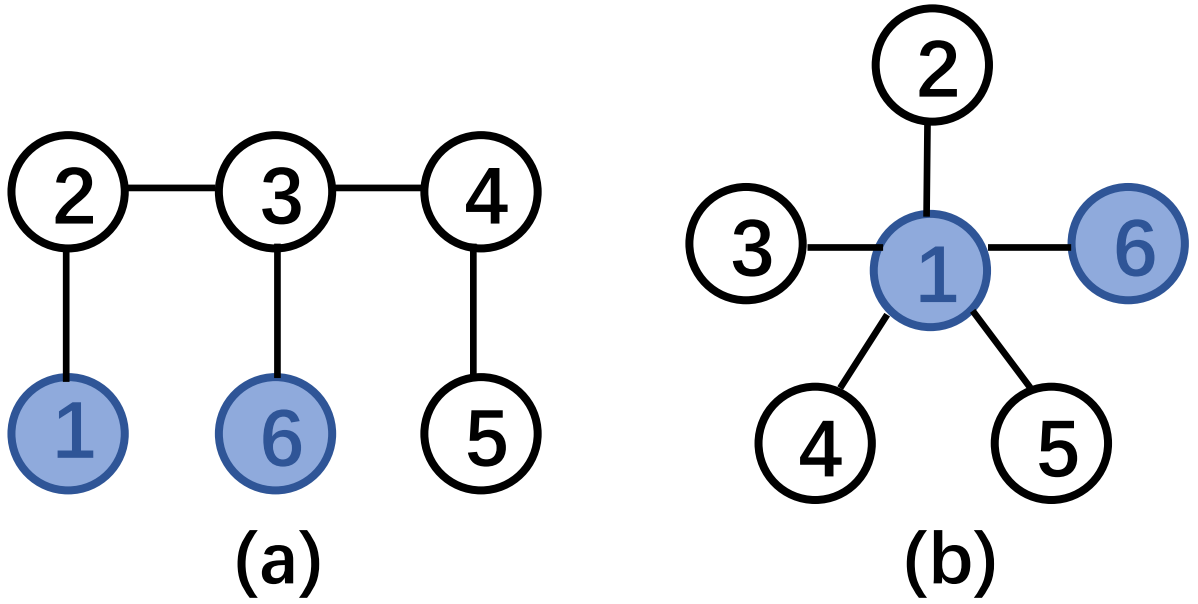
Node Distinguishability of Spectral GNNs

The Paradox

Despite highly parameterized graph filters, spectral GNNs assign *identical* embeddings to node 1 and 6.

The Culprit

Fixed graph matrices (normalized adjacency/Laplacian matrix) cause a fundamental loss of resolution in eigenspace due to the repeated eigenvalues and missing frequency components.



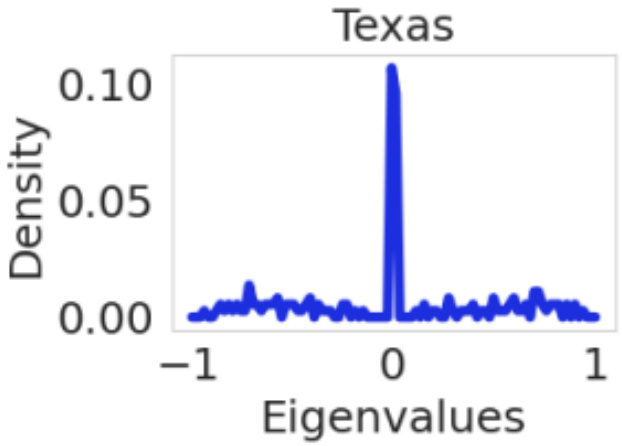
For graph signal $x = [1,0,0,0,0,1]$ and normalized adjacency matrix $\tilde{A}$, 1-order spectral GNNs *cannot distinguish* node 1 and 6.

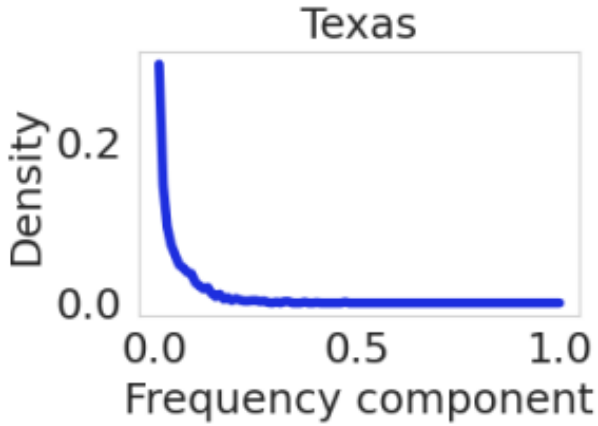
Lower Bound of Distinguished Nodes

Factor 1: Distinct Eigenvalues
The number of distinct eigenvalues in the graph matrix.
Graph symmetry reduces this.

$$\min\left(d_M, |\widetilde{X^{(M)}}|_0\right)$$

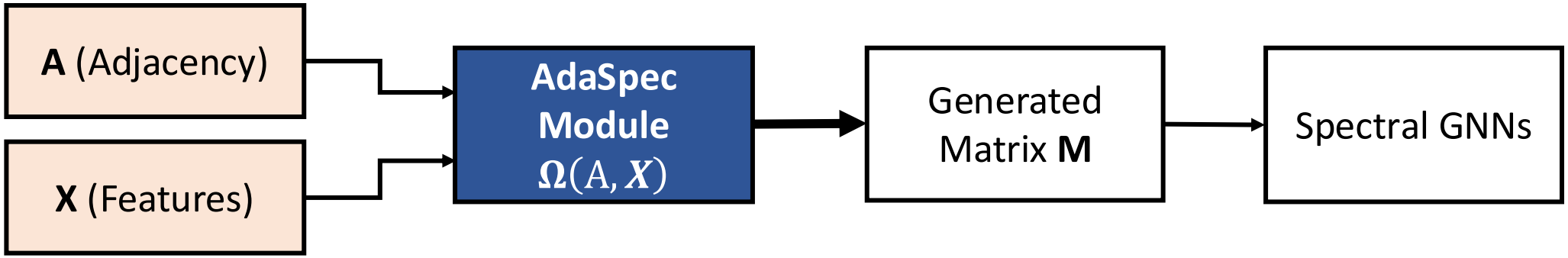
Factor 2: Non-zero Frequencies
The non-zero frequency components of node feature in the eigenspace.
Real-world sparsity drives this to zero.





Insight: Increase two variables for enhanced node distinguishability.

AdaSpec: An Adaptive, Plug-in Module



GNNs: $\Psi(M, X) = g_\Theta(M) f_W(X)$

$$M = \Omega(A, X) = \Omega_D(A) + \alpha_1 \Omega_S(A) + \alpha_2 \Omega_F(X)$$

$\Omega_D(A)$(Distinct Eigenvalues)

Uses a learnable bias **B** to break structural symmetry and increase distinct eigenvalues.

$\Omega_S(A)$(Shit from Zero)

Adds an identity matrix to shift eigenvalues from zero.

$\Omega_F(X)$(Frequency Components)

Adapts to node features to increase frequency components.

Experimental Results

The Setup

Evaluated across 18 benchmark datasets and 5 standard spectral GNNs (ChebNet, ChebNetII, JacobiConv, GPRGNN, BernNet)

The Breakthrough

Massive gains on complex heterophilic graphs where standard fixed graph matrix fail.

Model	Texas	Wisconsin	Actor	Chameleon	Squirrel	Cornell	Minesweeper	Questions
ChebNet(O)	38.67±9.31	32.92±7.38	25.15±0.69	29.32±4.13	24.23±3.24	31.33±7.51	86.29±0.2	55.13±0.54
ChebNet(M)	51.16±8.56	33.83±9.38	25.38±0.67	29.73±3.3	23.2±3.94	33.47±7.92	86.7±0.23	55.2±1.52
Δ ↑	+12.49	+0.91	+0.23	+0.41	-1.03	+2.14	+0.41	+0.07
ChebNetII(O)	56.24±1.39	51.5±5.63	29.89±0.68	35.26±3.66	37.19±0.66	39.54±6.88	78.35±0.14	64.13±0.95
ChebNetII(M)	56.76±3.12	52.0±7.75	30.43±1.23	35.62±3.52	36.88±0.69	39.94±7.05	79.1±0.09	65.54±0.7
Δ ↑	+0.52	+0.5	+0.54	+0.36	-0.31	+0.4	+0.75	+1.41
JacobiConv(O)	55.09±5.95	49.0±10.51	32.15±0.77	34.29±3.82	29.29±1.99	38.96±8.79	87.34±0.12	64.72±0.38
JacobiConv(M)	57.4±3.93	52.33±8.88	32.52±0.75	38.16±1.18	31.35±1.68	41.62±10.06	89.13±0.1	65.8±0.18
Δ ↑	+2.31	+3.33	+0.37	+3.87	+2.06	+2.66	+1.79	+1.08
GPRGNN(O)	48.15±4.74	44.25±5.92	30.39±1.24	32.5±2.92	27.7±3.88	34.39±6.88	87.15±0.49	53.14±0.27
GPRGNN(M)	58.27±4.97	53.25±7.21	30.4±1.51	32.82±4.76	27.3±6.03±4.77	36.13±7.52	88.58±0.18	58.19±0.36
Δ ↑	+10.12	+9.0	+0.01	+0.32	-0.4	+1.74	+1.43	+5.05
BernNet(O)	56.19±7.52	49.38±5.75	30.5±1.18	35.35±3.46	33.41±3.42	36.82±10.64	76.54±0.23	64.86±0.37
BernNet(M)	58.9±4.11	51.96±7.84	30.61±0.67	39.61±1.55	34.46±3.52	40.23±5.66	76.95±0.21	65.2±0.31
Δ ↑	+2.71	+2.58	+0.11	+4.26	+1.05	+3.41	+0.41	+0.34

Performance of spectral GNNs with/without AdaSpec on heterophilic datasets. ROC AUC is reported on Minesweeper, Questions. Testing accuracy is reported on other datasets. High value indicate good performance.

Computational Complexity: Zero Asymptotic Overhead

Pre-computation

There is a one-time pre-computation before training in order $O\big(h(|\mathcal{V}| + |\mathcal{E}|)\big)$. On massive graphs like Coauthor-Physics, the one-time pre-computation takes only 12.44 seconds.

Forward/Backward Complexity

The asymptotic order remains the same during training phase.

Spectral GNNs	Parameter Count	Pre-computing Complexity	Forward/Backward Complexity
$\Psi(M, X)$	$1 + K$	$O(\|\mathcal{V}\| + \|\mathcal{E}\|)$	$O(KT\|\mathcal{E}\| + \|\mathcal{V}\|\|W\|)$
$\Psi^{+}(A, X)$	$1 + K + \|\mathcal{V}\|$	$O(h(\|\mathcal{V}\| + \|\mathcal{E}\|))$	$O(KT\|\mathcal{E}\| + \|\mathcal{V}\|\|W\|)$

Time complexity comparison of GNNs with/without AdaSpec. $\mathcal{V}$ and $\mathcal{E}$ denotes the node and edge set respectively. h is the node feature dimension. T is the node class number. K is the polynomial orders of spectral GNNs.

Conclusion and Future Work

- **Key Insight:** Node distinguishability in spectral GNNs is driven by the interaction between **eigenvalue diversity** and **node feature frequency components**.

- **The Solution:** Introduces **AdaSpec**, a plug-and-play module that provides theoretical guarantees for enhanced distinguishability and consistent empirical performance gains.

- **Next Steps:** Future research will focus on generalizing the module for **dynamic graphs** and broader data distributions.