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# Spectral Pruning Can Mitigate Over-squashing and Over-smoothing in Graph Neural Networks

*Adarsh Jamadandi, Celia Rubio-Madrigal, and Rebekka Burkholz.*
*CISPA, Saarland University.*

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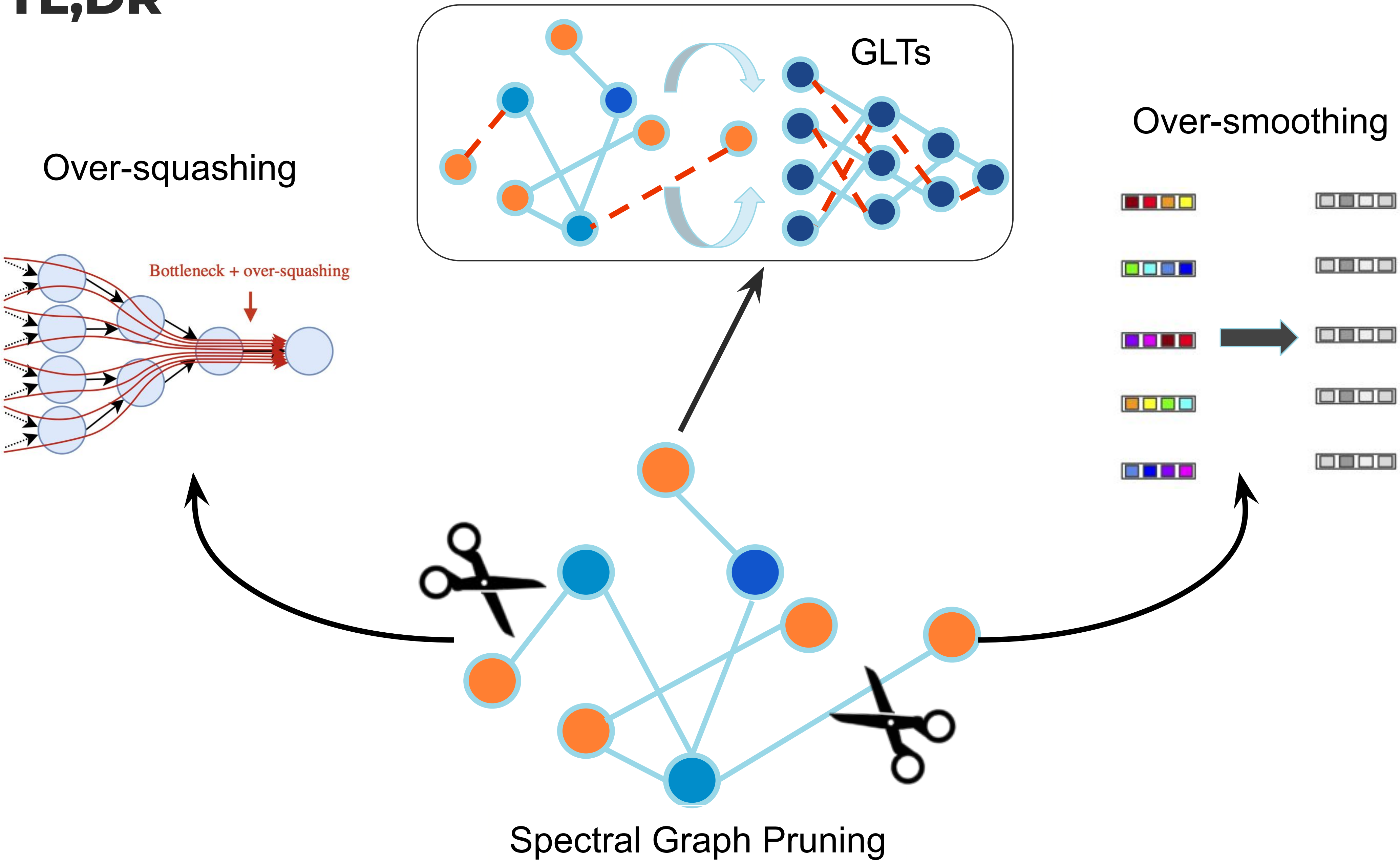
# TL;DR

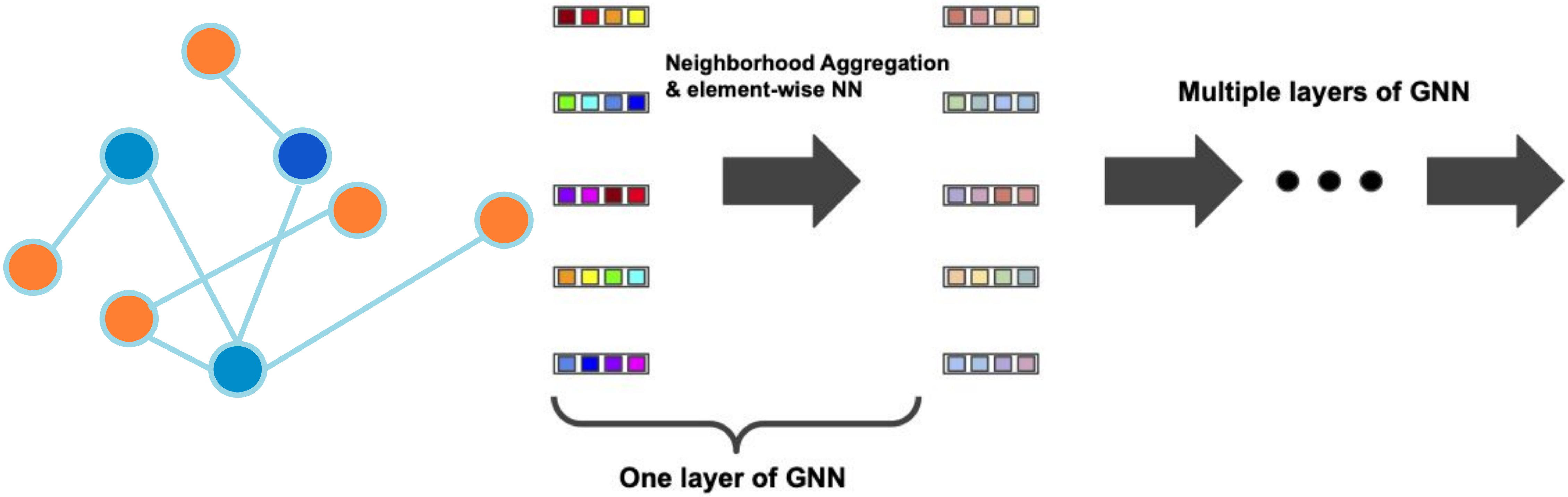


GLTs
Over-squashing
Bottleneck + over-squashing
Over-smoothing
Spectral Graph Pruning

# Graph Neural Networks

- Graph Neural Networks aggregate vector based information on the graph, aka message-passing.

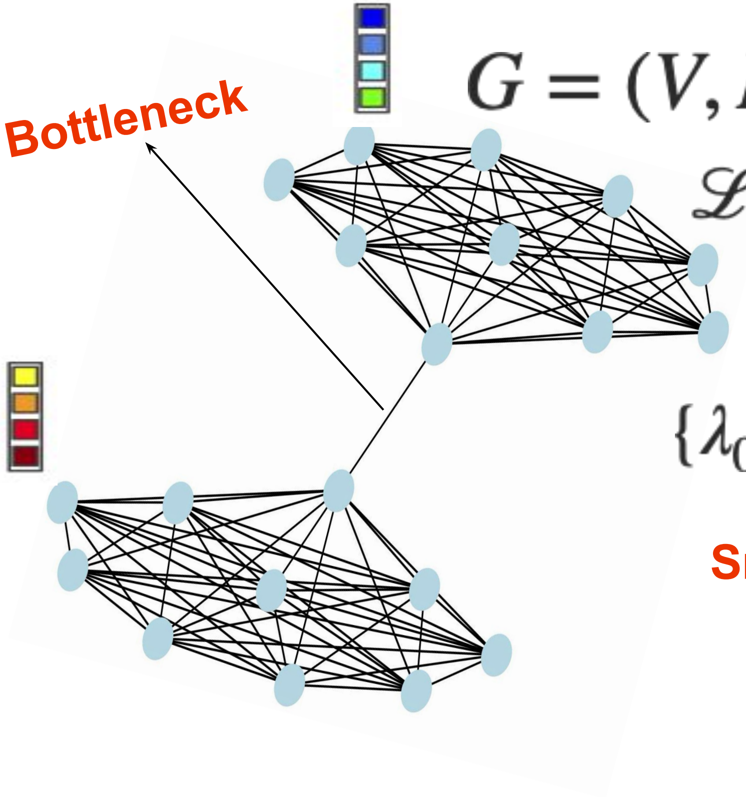
- What are the factors that could affect the efficiency of message passing?



# Over-squashing and Over-smoothing

- How to balance over-squashing and over-smoothing?

**Over-squashing**



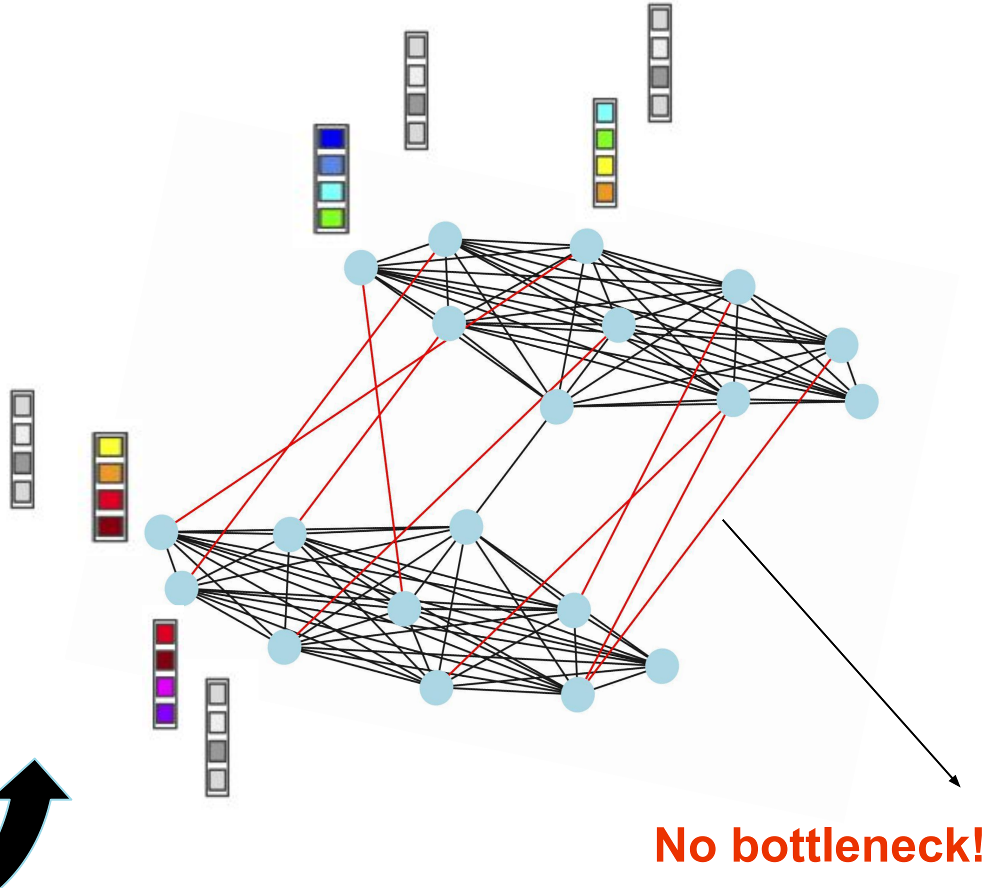

$$G = (V, E)$$

$$\mathscr{L}_G = D^{-1/2} \mathscr{L} D^{-1/2}$$

$$\{\lambda_0 < \lambda_1 < \lambda_2, \ldots \lambda_n\}$$

**Small spectral gap**

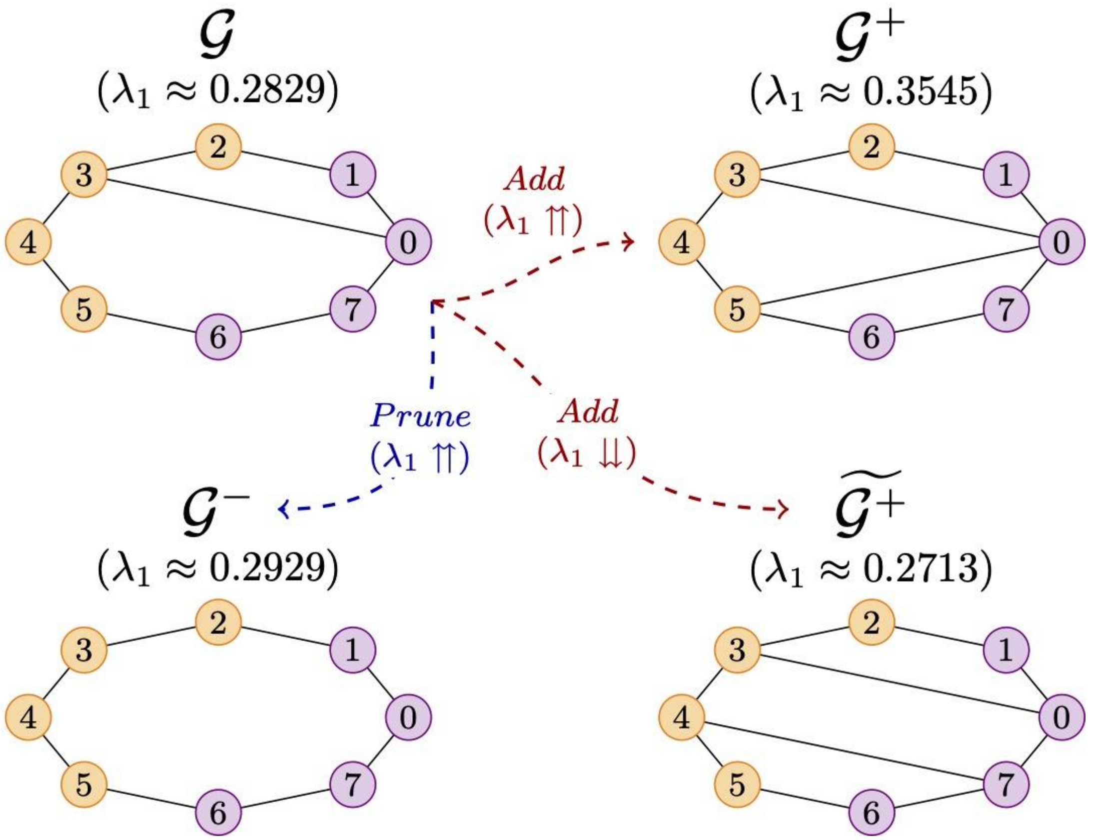
**Over-smoothing**

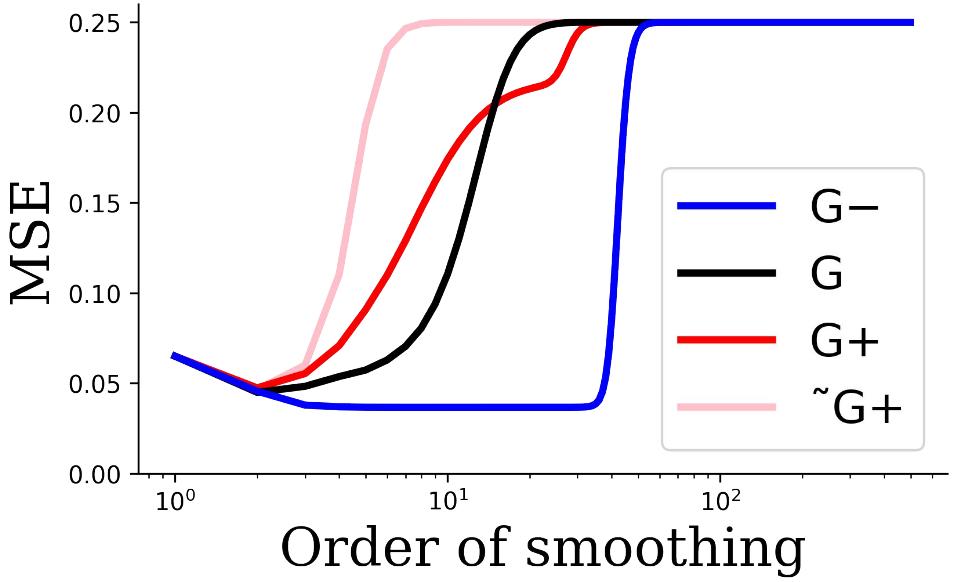


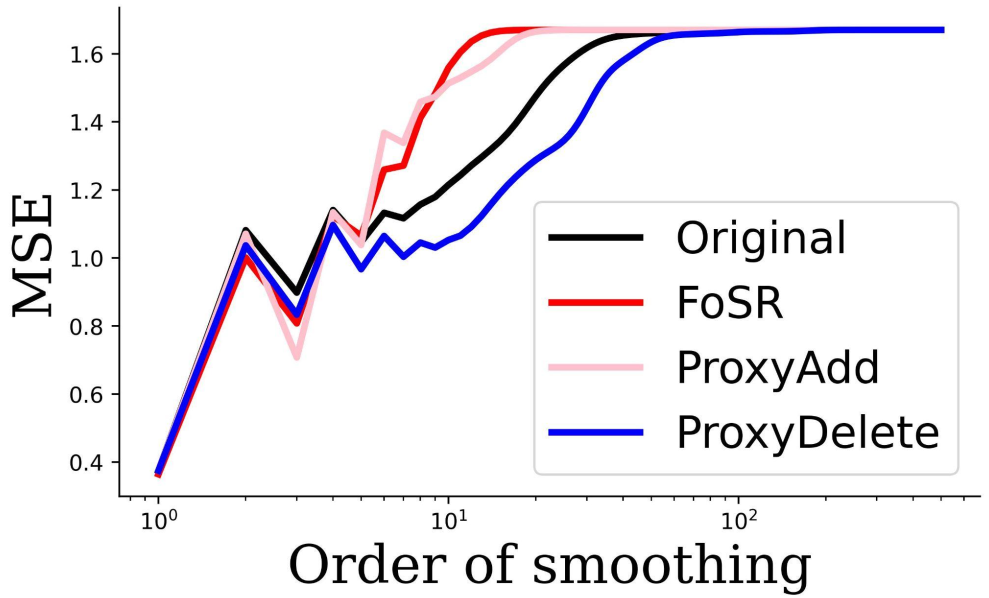
# Braess Paradox to the Rescue!

Adding an extra road causes delays!

# Braess Paradox and Spectral Pruning



# Braess criterion and Proxy spectral gap

**Lemma 2.1.** *Eldan et al. (2017): Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a finite graph, with $f$ denoting the eigenvector and $\lambda_1(\mathcal{L}_\mathcal{G})$ the eigenvalue corresponding to the spectral gap. Let $\{u, v\} \notin \mathcal{V}$ be two vertices that are not connected by an edge. Denote $\hat{\mathcal{G}} = (\mathcal{V}, \hat{\mathcal{E}})$, the new graph obtained after adding an edge between $\{u, v\}$, i.e., $\hat{\mathcal{E}} := \mathcal{E} \cup \{u, v\}$. Denote with $\mathcal{P}_f := \langle f, \hat{f}_0 \rangle$ the projection of $f$ onto the top eigenvector of $\hat{\mathcal{G}}$. Define $g(u, v, \mathcal{L}_\mathcal{G}) :=$*

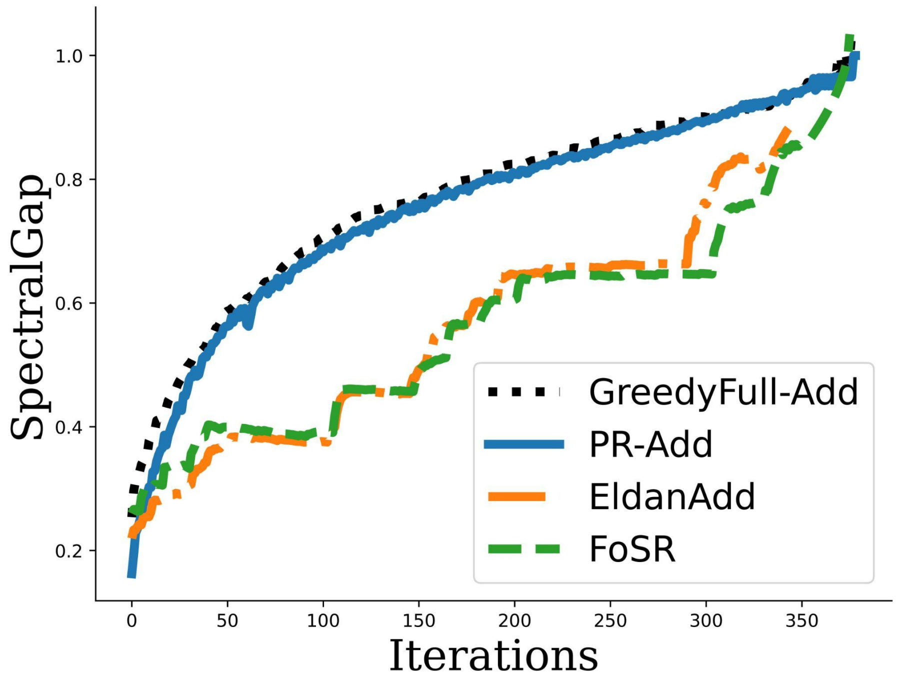
$$-\mathcal{P}_f^2 \lambda_1(\mathcal{L}_\mathcal{G}) - 2(1 - \lambda_1(\mathcal{L}_\mathcal{G})) \left( \frac{\sqrt{d_u + 1} - \sqrt{d_u}}{\sqrt{d_u + 1}} f_u^2 + \frac{\sqrt{d_v + 1} - \sqrt{d_v}}{\sqrt{d_v + 1}} f_v^2 \right) + \frac{2 f_u f_v}{\sqrt{d_u + 1}\sqrt{d_v + 1}}.$$

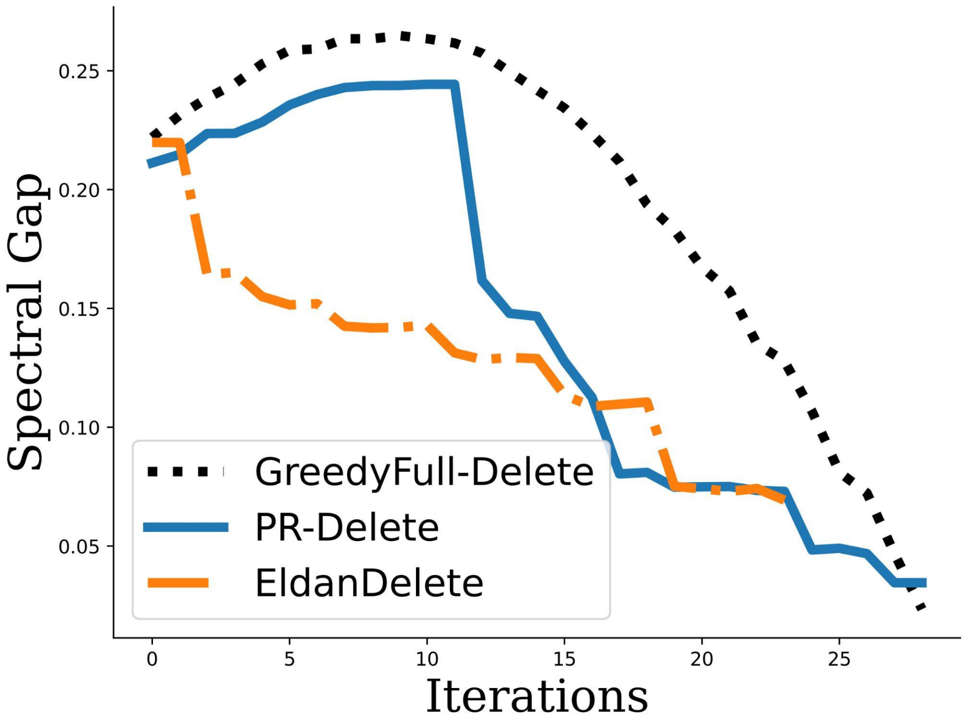
*If $g(u, v, \mathcal{L}_\mathcal{G}) > 0$, then $\lambda_1(\mathcal{L}_\mathcal{G}) > \lambda_1(\mathcal{L}_{\hat{\mathcal{G}}})$.*

## Proxy Spectral Gap

$$\acute{\lambda} \approx \lambda + \Delta w_{u,v}((f_u - f_v)^2 - \lambda(f_u^2 + f_v^2)),$$

# How good is this proxy?




| Method | Cora | Citeseer | Chameleon | Squirrel |
|---|---|---|---|---|
| FoSR | 4.69 | 5.33 | 5.04 | 19.48 |
| SDRF | 19.63 | 173.92 | 17.93 | 155.95 |
| PROXYADD | 4.30 | 3.13 | 1.15 | 9.12 |
| PROXYDELETE | 1.18 | 0.86 | 1.46 | 7.26 |

# Results

Table 2: Results on Long Range Graph Benchmark datasets.

| Method | PascalVOC-SP ( Test F1 ↑) | Peptides-Func (Test AP ↑) | Peptides-Struct (Test MAE ↓) |
|---|---|---|---|
| Baseline-GCN | 0.1268±0.0060 | 0.5930±0.0023 | 0.3496±0.0013 |
| DRew+GCN | 0.1848±0.0107 | **0.6996±0.0076** | 0.2781±0.0028 |
| ProxyAdd+GCN | **0.2213±0.0011** | 0.6789±0.0002 | **0.2465±0.0004** |
| ProxyDelete+GCN | **0.2170±0.0015** | 0.6908±0.0007 | **0.2470±0.0080** |

Table 3: Node classification on Amazon-Ratings.

| Method | #EdgesAdded | Accuracy | #EdgesDeleted | Accuracy | Layers |
|---|---|---|---|---|---|
| GCN | - | 47.20±0.33 | - | 47.20±0.33 | 10 |
| GCN+FoSR | 25 | 49.68±0.73 | - | - | 10 |
| GCN+Eldan | 25 | 48.71±0.99 | 100 | **50.15±0.50** | 10 |
| GCN+ProxyGap | 10 | 49.72±0.41 | 50 | **49.75±0.46** | 10 |
| GAT | - | 47.43±0.44 | - | 47.43±0.44 | 10 |
| GAT+FoSR | 25 | 51.36±0.62 | - | - | 10 |
| GAT+Eldan | 25 | 51.68±0.60 | 50 | **51.80±0.27** | 10 |
| GAT+ProxyGap | 20 | 49.06±0.92 | 100 | **51.72±0.30** | 10 |
| GCN | - | 47.32±0.59 | - | 47.32±0.59 | 20 |
| GCN+FoSR | 100 | 49.57±0.39 | - | - | 20 |
| GCN+Eldan | 50 | **49.66±0.31** | 20 | 48.32±0.76 | 20 |
| GCN+ProxyGap | 50 | 49.48±0.59 | 500 | **49.58±0.59** | 20 |
| GAT | - | 47.31±0.46 | - | 47.31±0.46 | 20 |
| GAT+FoSR | 100 | 51.31±0.44 | - | - | 20 |
| GAT+Eldan | 20 | 51.40±0.36 | 20 | **51.64±0.44** | 20 |
| GAT+ProxyGap | 50 | 47.53±0.90 | 20 | **51.69±0.46** | 20 |

Table 4: Node classification on Minesweeper.

| Method | #EdgesAdded | Accuracy | #EdgesDeleted | Test ROC | Layers |
|---|---|---|---|---|---|
| GCN | - | 88.57± 0.64 | - | 88.57± 0.64 | 10 |
| GCN+FoSR | 50 | 90.15±0.55 | - | - | 10 |
| GCN+Eldan | 100 | **90.11±0.50** | 50 | 89.49±0.60 | 10 |
| GCN+ProxyGap | 20 | **89.59±0.50** | 20 | 89.57±0.49 | 10 |
| GAT | - | 93.60±0.64 | - | 93.60±0.64 | 10 |
| GAT+FoSR | 100 | 93.14±0.43 | - | - | 10 |
| GAT+Eldan | 50 | 93.26±0.48 | 100 | **93.82±0.56** | 10 |
| GAT+ProxyGap | 20 | 93.60±0.69 | 20 | **93.65±0.84** | 10 |
| GCN | - | 87.41±0.65 | - | 87.41±0.65 | 20 |
| GCN+FoSR | 100 | 89.64±0.55 | - | - | 20 |
| GCN+Eldan | 72 | **89.70±0.57** | 10 | 88.90±0.44 | 20 |
| GCN+ProxyGap | 20 | **89.46±0.50** | 50 | 89.35±0.30 | 20 |
| GAT | - | 93.92±0.52 | - | 93.92±0.52 | 20 |
| GAT+FoSR | 50 | 93.56±0.64 | - | - | 20 |
| GAT+Eldan | 10 | 93.92±0.44 | 20 | **95.48±0.64** | 20 |
| GAT+ProxyGap | 20 | **94.89±0.67** | 20 | 94.64±0.81 | 20 |

# Results

Table 3: Pruning for lottery tickets comparing UGS to our ELDANDELETE pruning and our PROXY-DELETE pruning. We report Graph Sparsity (GS), Weight Sparsity (WS), and Accuracy (Acc).

| Method | Cora | | | Citeseer | | | Pubmed | | |
|---|---|---|---|---|---|---|---|---|---|
| Metrics | GS | WS | Acc | GS | WS | Acc | GS | WS | Acc |
| UGS | 79.85% | 97.86% | 68.46±1.89 | 78.10% | 97.50% | **66.50±0.60** | 68.67% | 94.52% | 76.90±1.83 |
| ELDANDELETE-UGS | 79.70% | 97.31% | 68.73±0.01 | 77.84% | 96.78% | 64.60±0.00 | 70.11% | 93.17% | **78.00±0.42** |
| PROXYDELETE-UGS | 78.81% | 97.24% | **69.26±0.63** | 77.50% | 95.83% | 65.43±0.60 | 78.81% | 97.24% | 75.25±0.25 |

# Summary

- Over-squashing and Over-smoothing not a trade-off.
- Spectral graph pruning can simultaneously mitigate both!
- Interesting application also find Graph Lottery Tickets!
- We propose a computationally friendly proxy method for spectral gap approximation.

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# References

- Aggregation steps visualization - https://disco.ethz.ch/courses/fs21/seminar/talks/GNN_Oversmoothing.pdf
- Bottleneck visualization - https://urialon.cswp.cs.technion.ac.il/wp-content/uploads/sites/83/2020/07/bottleneck_slides.pdf
- Braess paradox city visualization - https://unsplash.com/@dnevozhai