

Learning Graph Neural Networks on Complex Structured Data

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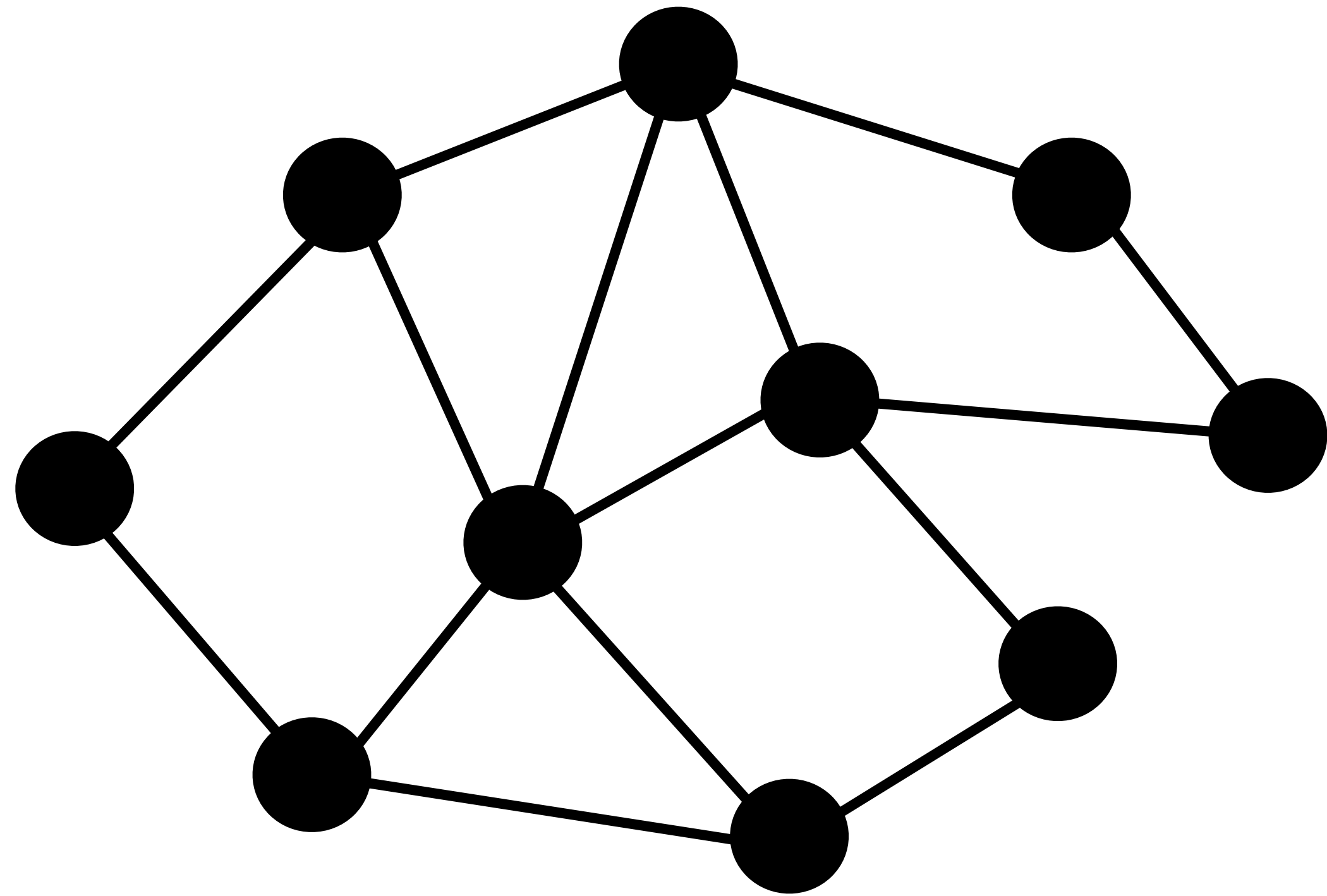
Prof. Rui Zhang



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- Research Background
- Motivation & Challenges
- Introduction of Proposed Works
- Conclusion & Future Work

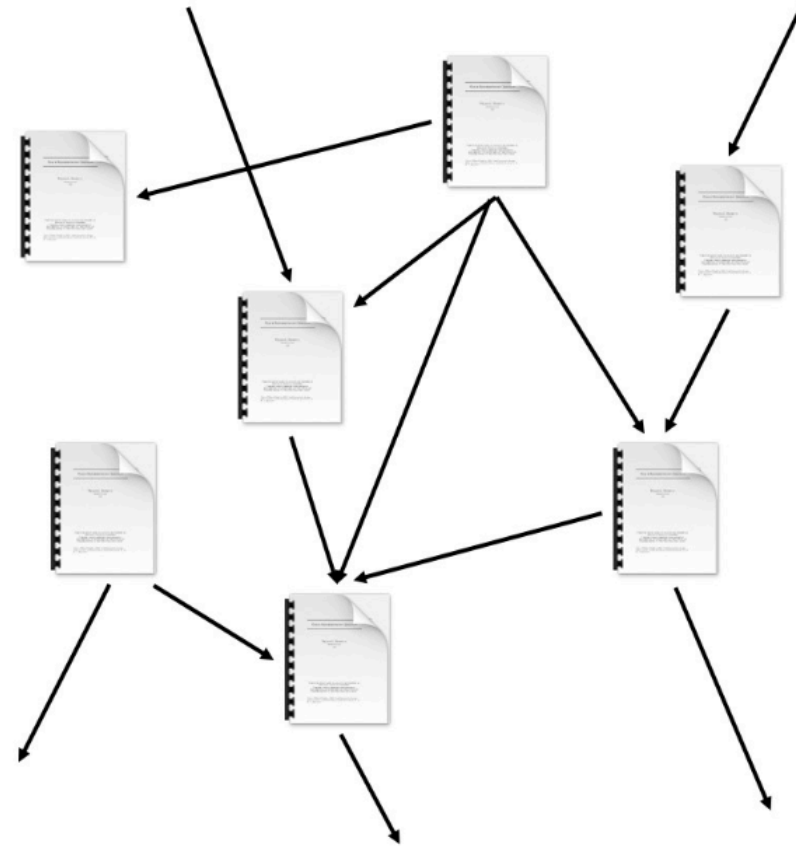
Background — What is Graph?



Graph

Graphs are a general language describing and analyzing **entities with relations or interactions.**

Background — Many Types of Data are Graphs



Citation Network



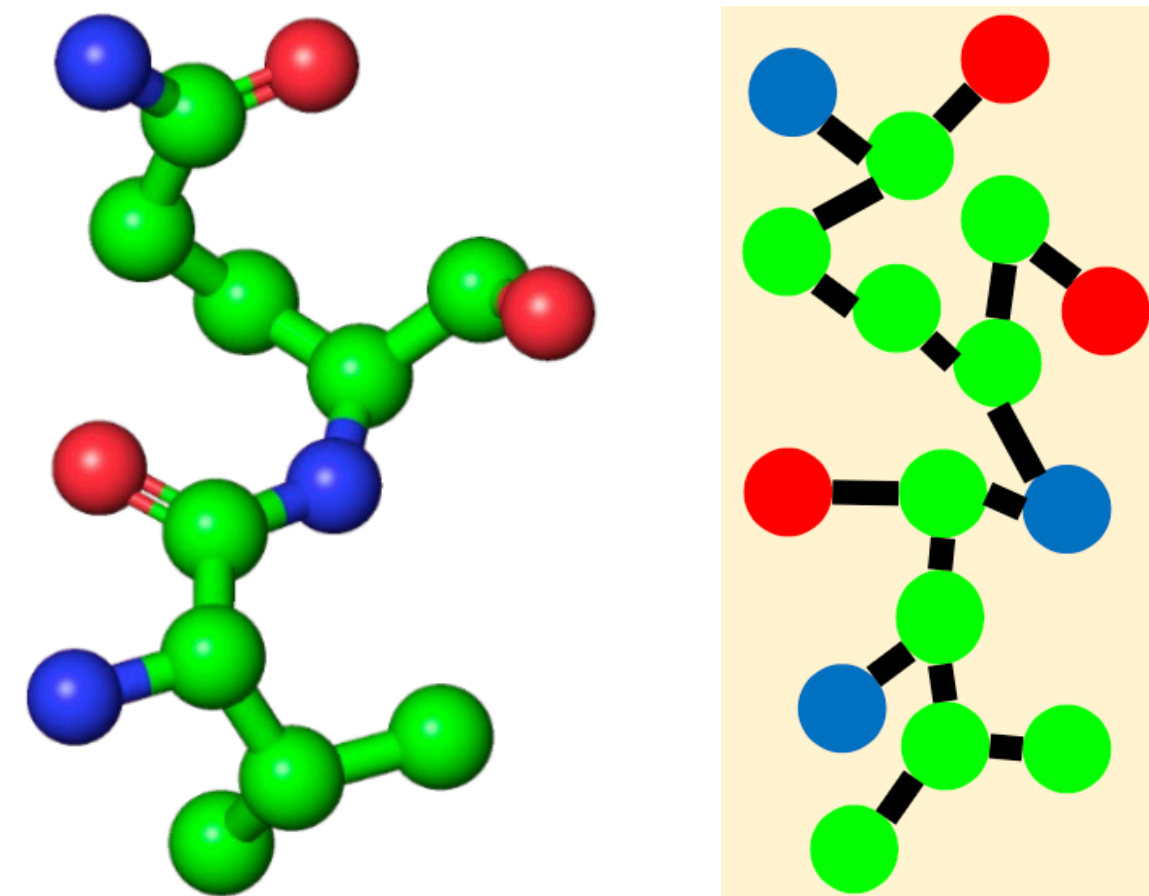
Social Network



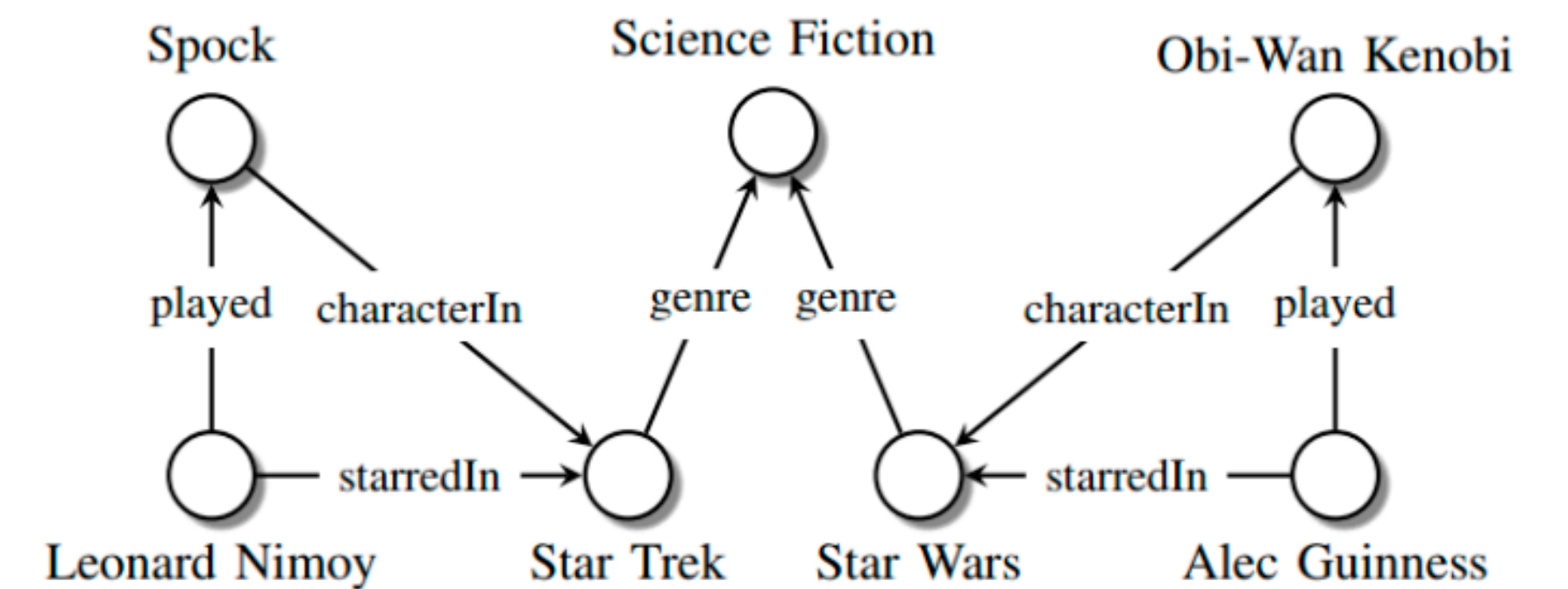
Internet (e.g., Webpage)



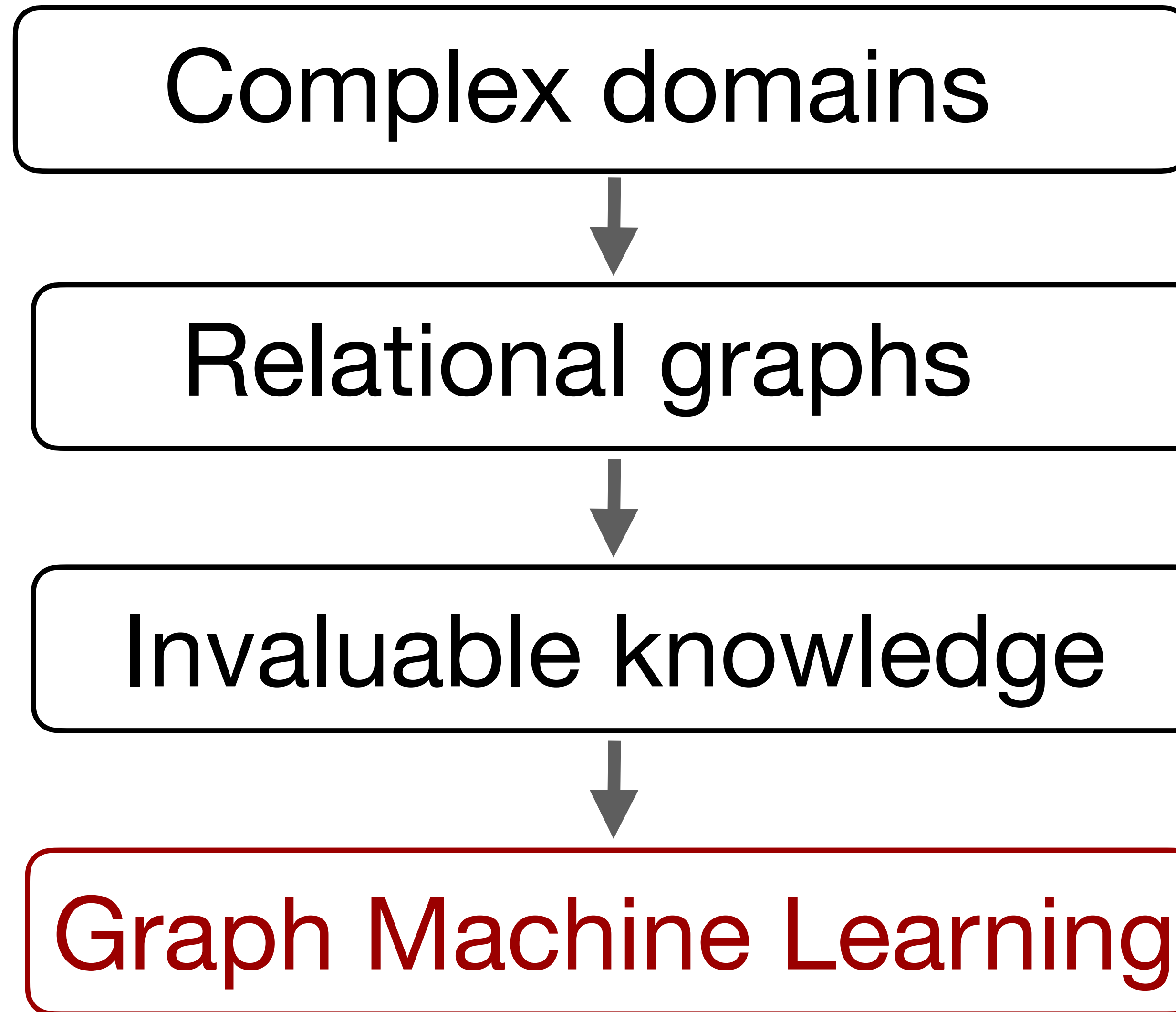
Brain Network



Molecules

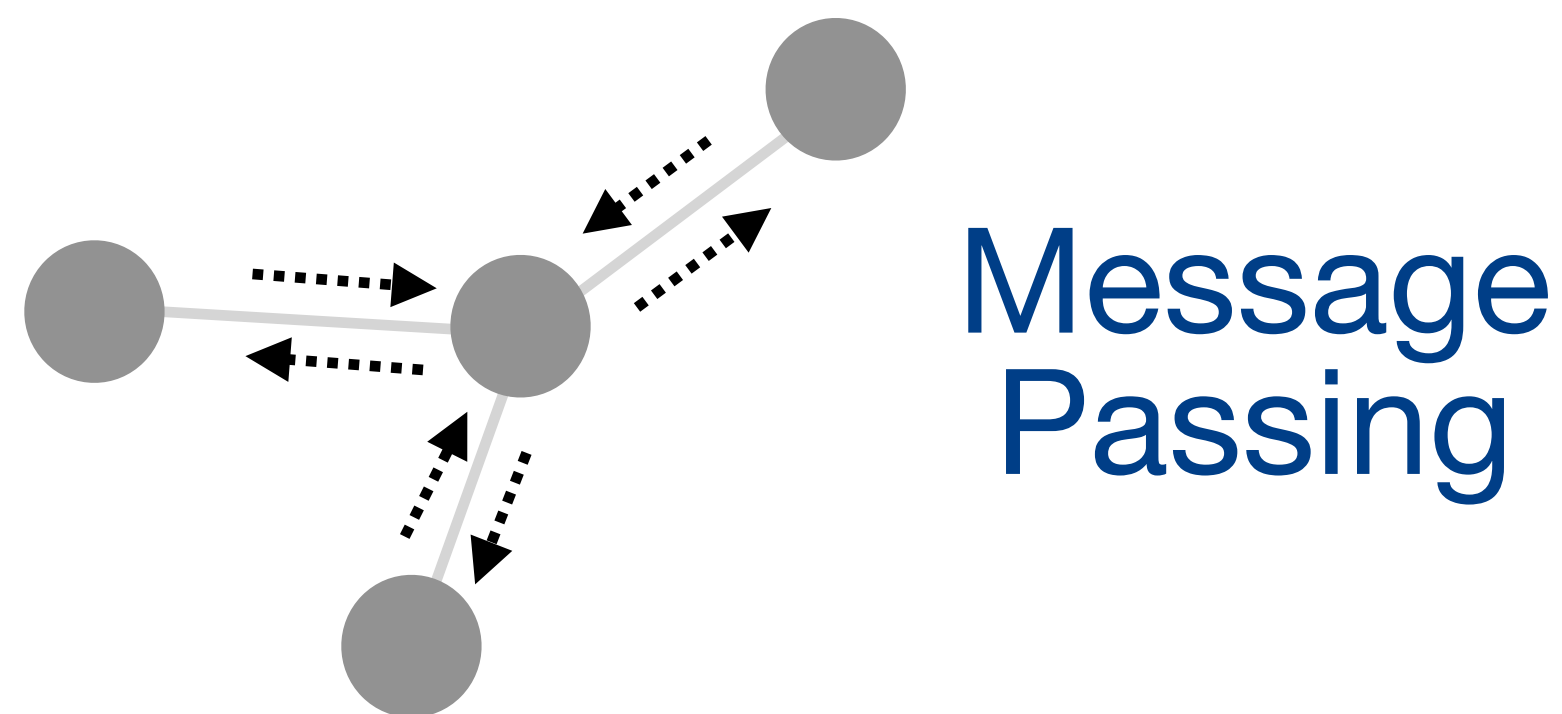


Knowledge Graph

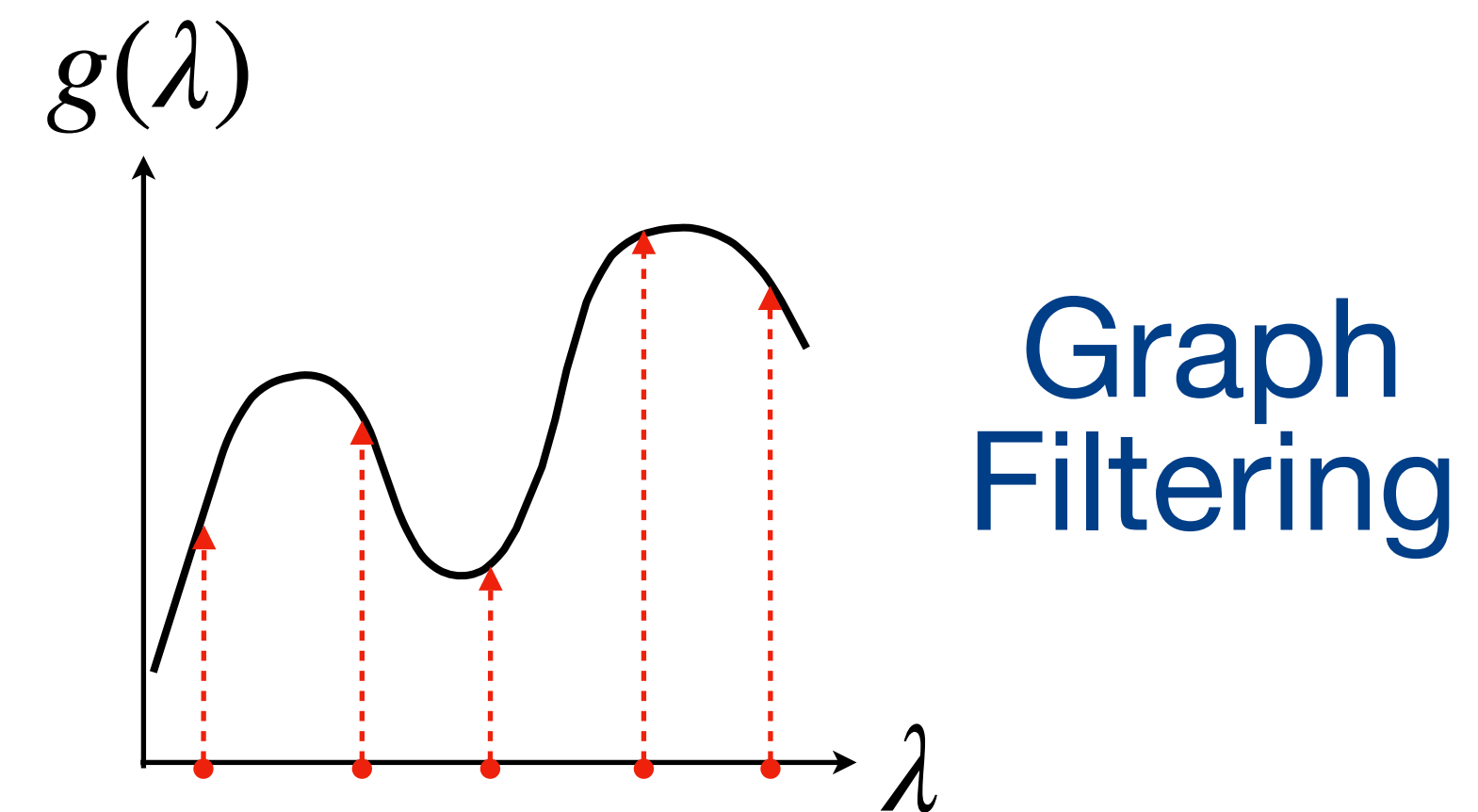


GNNs integrate both node features and graph topology via either a **message passing framework** or a **graph filtering operation**.

■ Spatial-based Methods



■ Spectral-based Methods



Background — Unified Framework of GNNs

Most GNNs can be interpreted as **different solutions to the same graph denoising problem:**

$$\arg \min_{\mathbf{Z}} \|\mathbf{Z} - \mathbf{X}\|_2^2 + \lambda \operatorname{tr}(\mathbf{Z}^T \hat{\mathbf{L}} \mathbf{Z})$$

↑
keep close to the
original features

↑
smooth node features
across the graph

Ma, Y., et.al. A unified view on graph neural networks as graph signal denoising. CIKM 2021.

Zhu, M., et.al. Interpreting and unifying graph neural networks with an optimization framework. WWW 2021.

Gasteiger, J., et.al. Predict then propagate: Graph neural networks meet personalized pagerank. ICLR 2019.

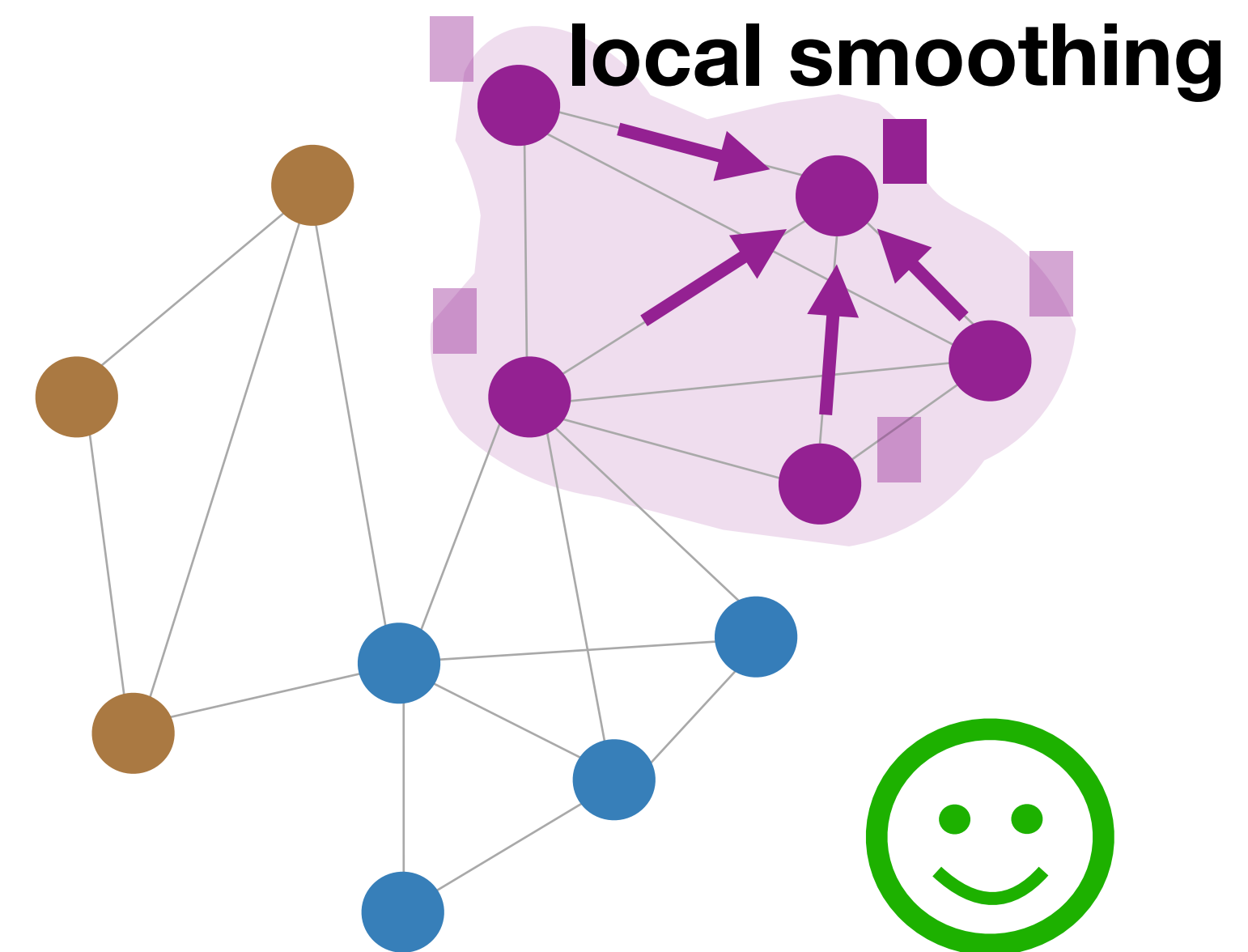
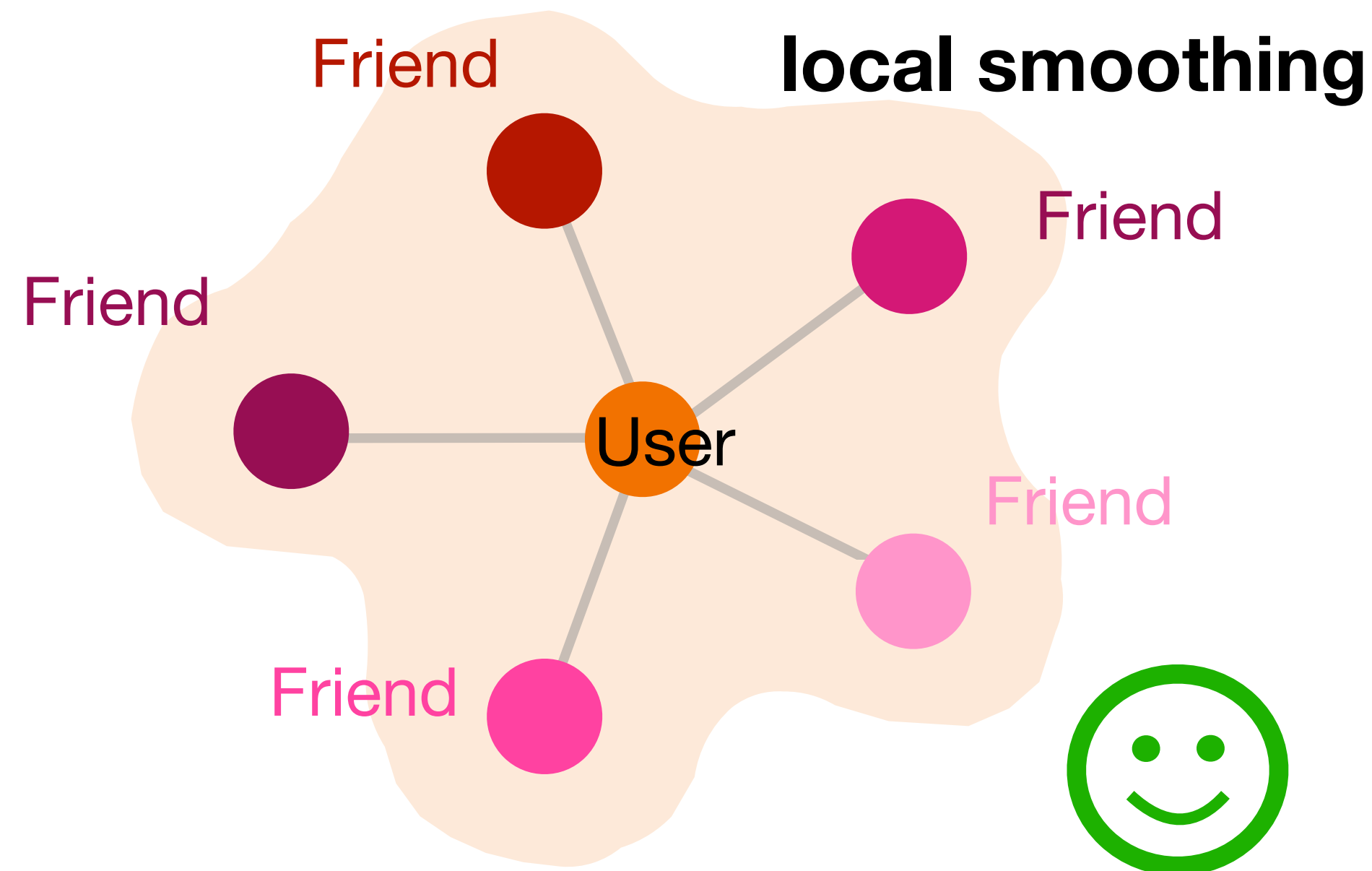
Veličković, P., et.al. Graph attention networks. ICLR 2018.

Kipf & Welling, Semi-supervised classification with graph convolutional networks. ICLR 2017.

Motivation — Smoothness Assumption in GNNs

Most GNNs implicitly **assume homogeneity in node interactions and smooth node neighborhood.**

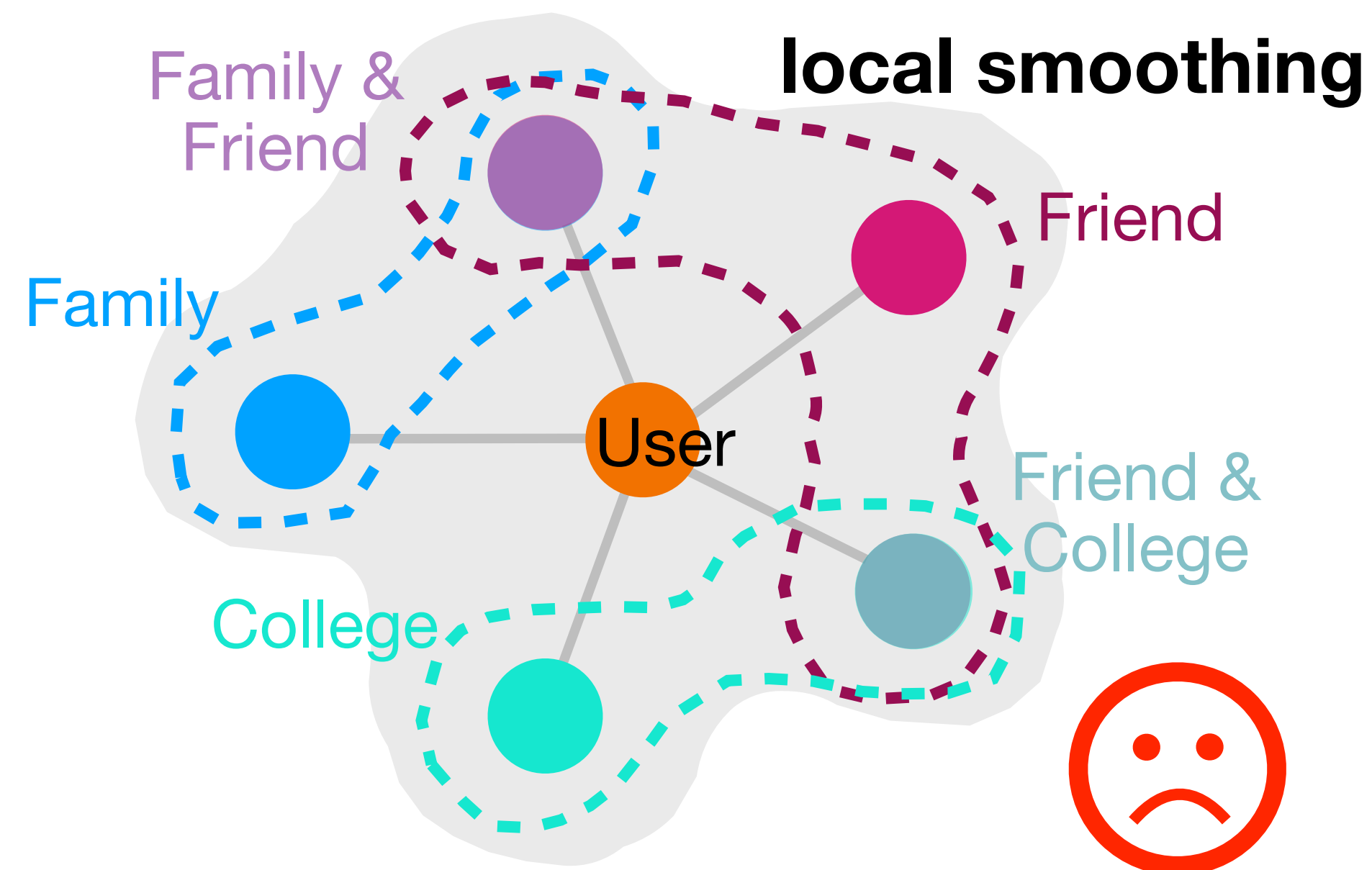
- Homogenous Node Relationships
- Homophilic Linking Patterns



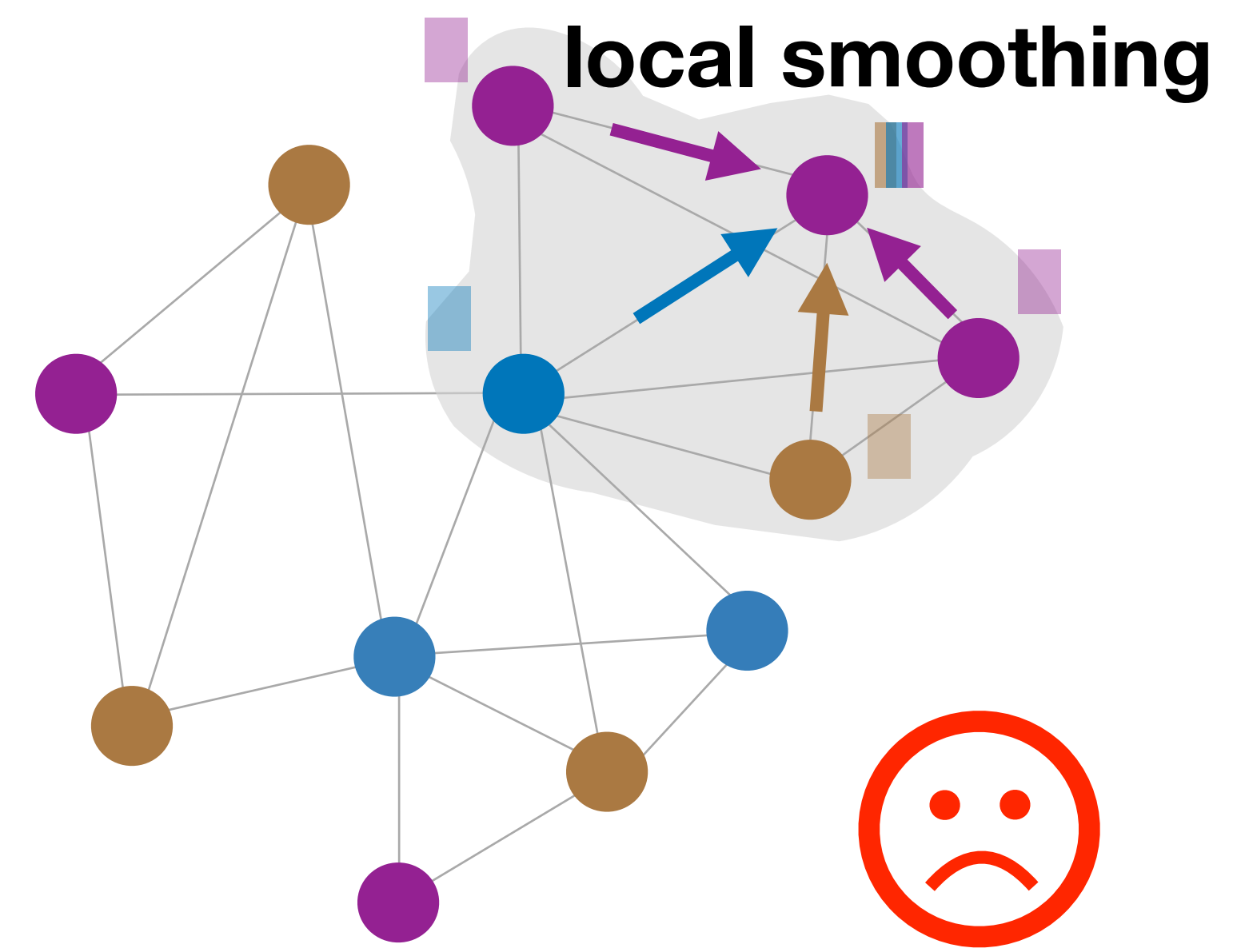
Challenges — Entangled Relationships & Heterophilic Links

Most GNNs implicitly **assume homogeneity in node interactions and smooth node neighborhood.**

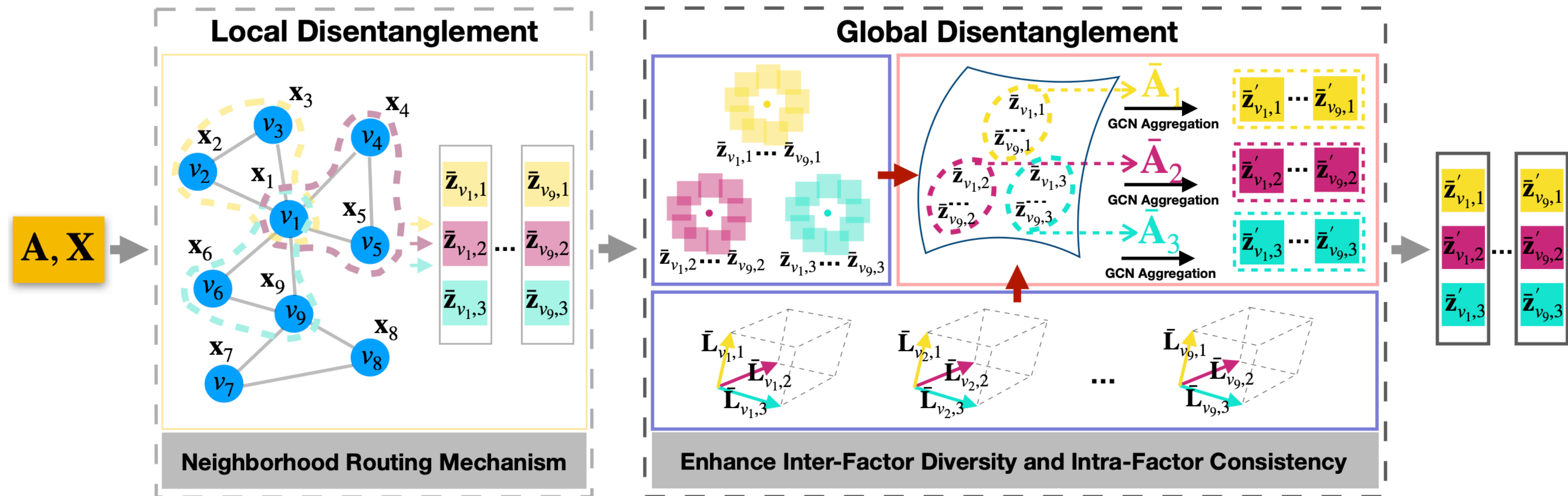
■ Entangled Node Relationships



■ Heterophilic Linking Patterns



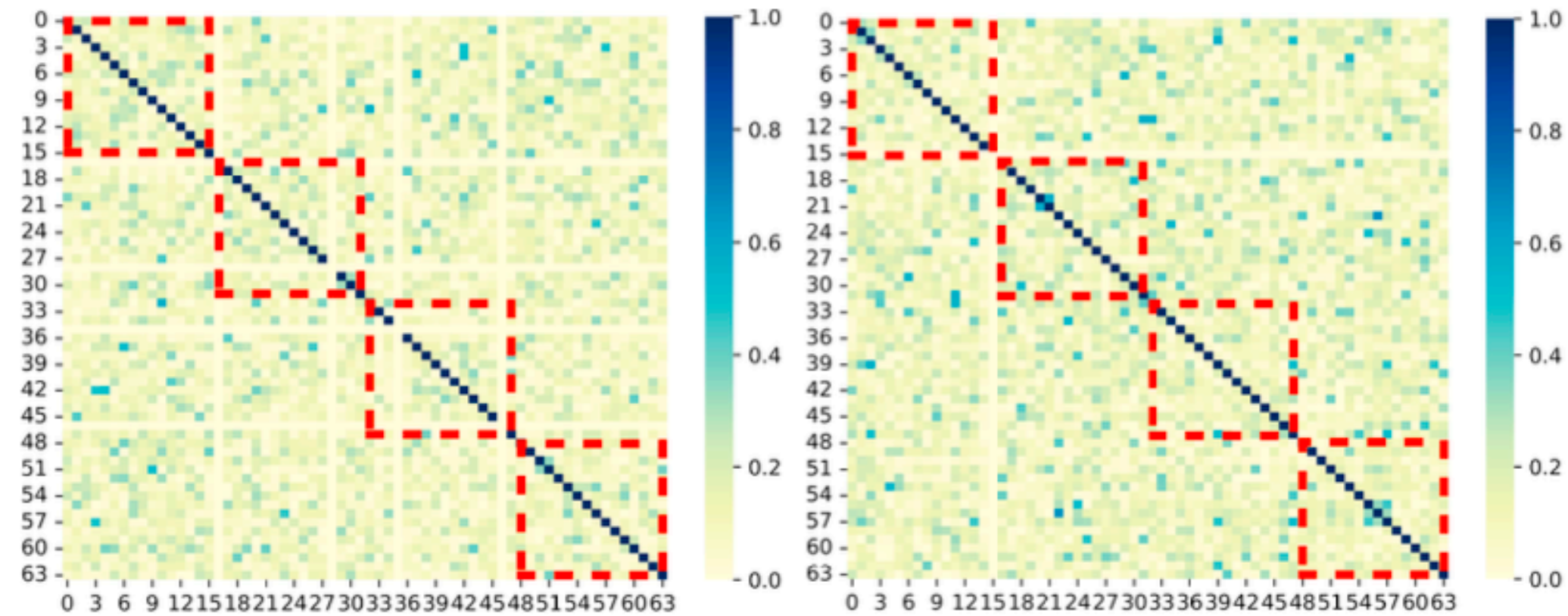
Proposed Works — Chapter 3: Local-Global Disentanglement



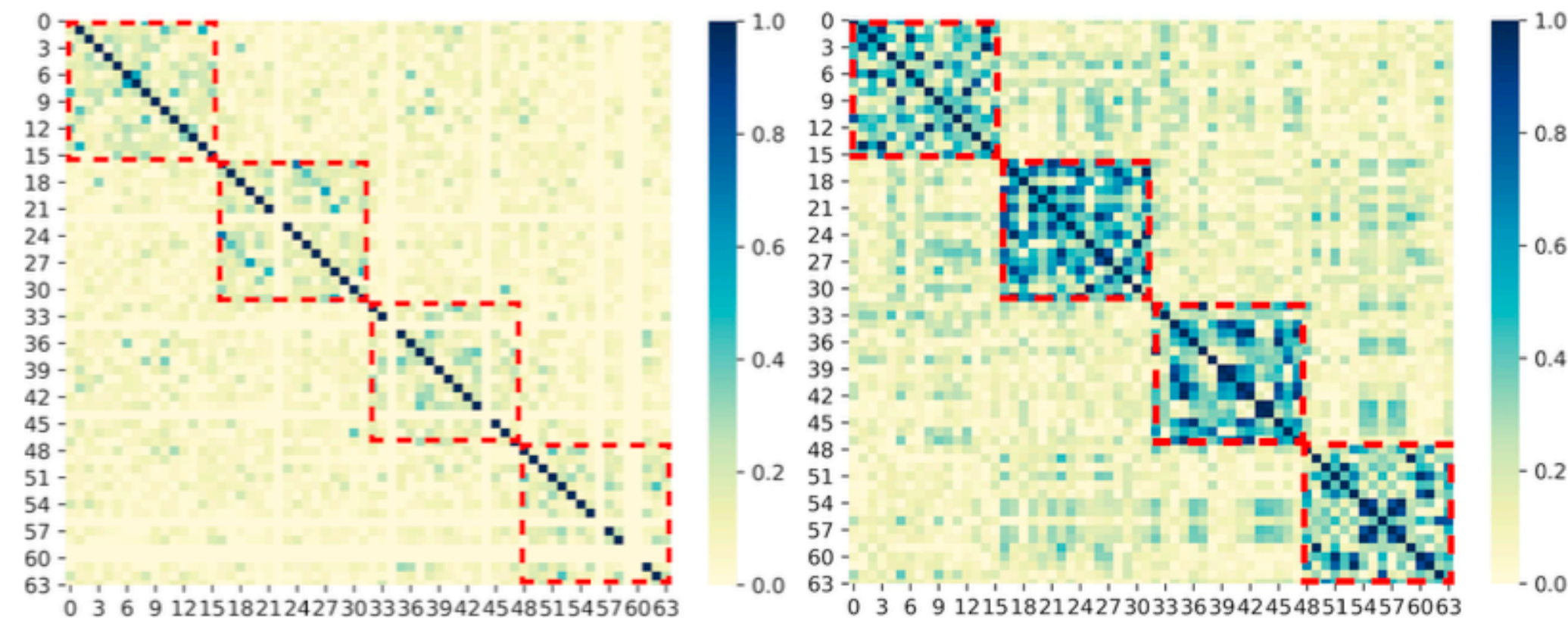
LGD incorporates both **local and global information** for graph disentanglement to address **entangled node relationships**.

Proposed Works — Chapter 3: Local-Global Disentanglement

Experimental Results



(a) DisenGCN (1st Layer) (b) DisenGCN (2nd Layer)



(c) LGD (1st Layer) (d) LGD (2nd Layer)

LGD can produce representations with a higher level of disentanglement.

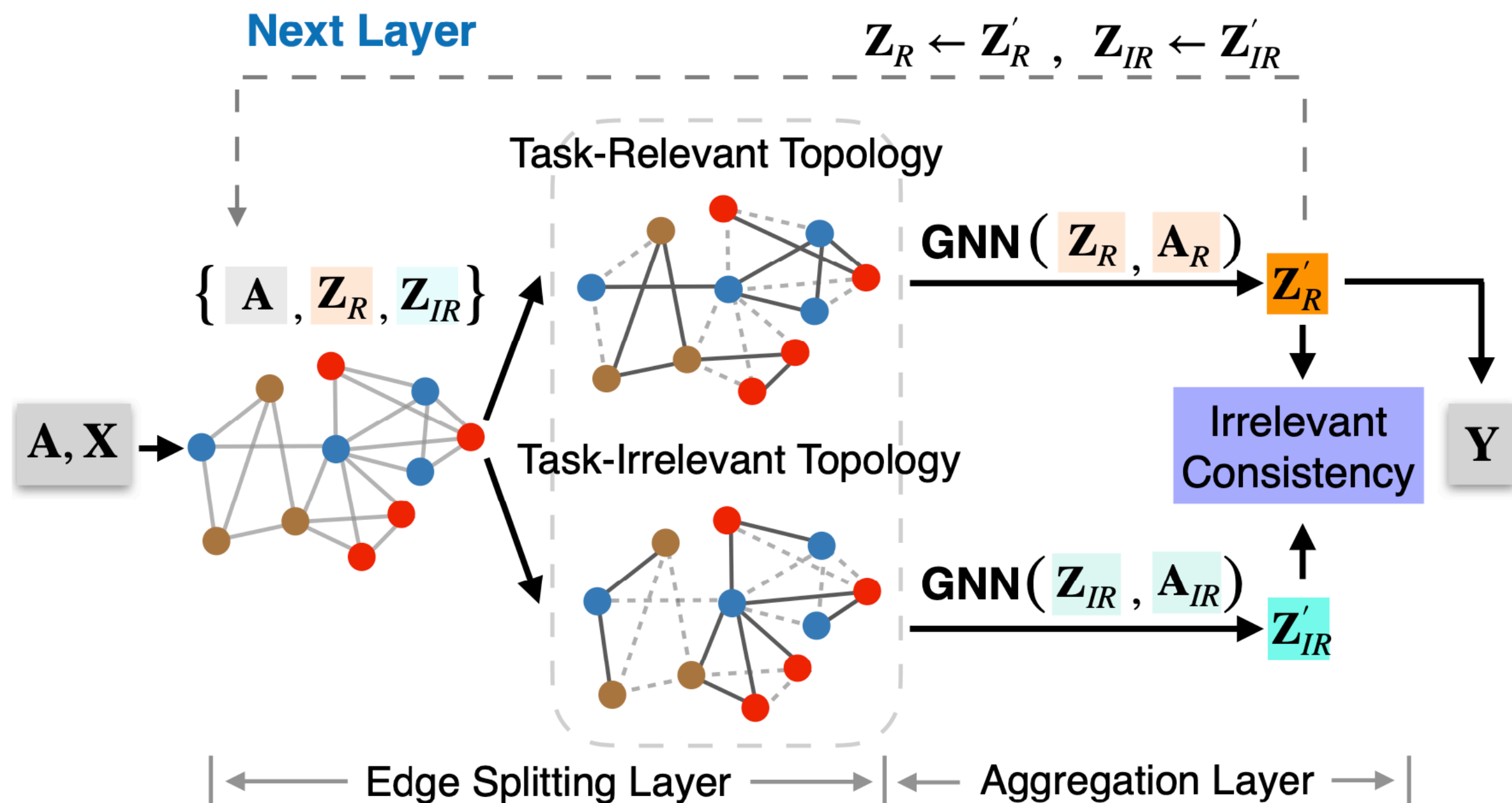
Proposed Works — Chapter 4: Edge Splitting GNN

Conventional Smoothness Assumption

Two connected nodes **mostly share task-beneficial similarity**.

Disentangled Smoothness Assumption (Ours)

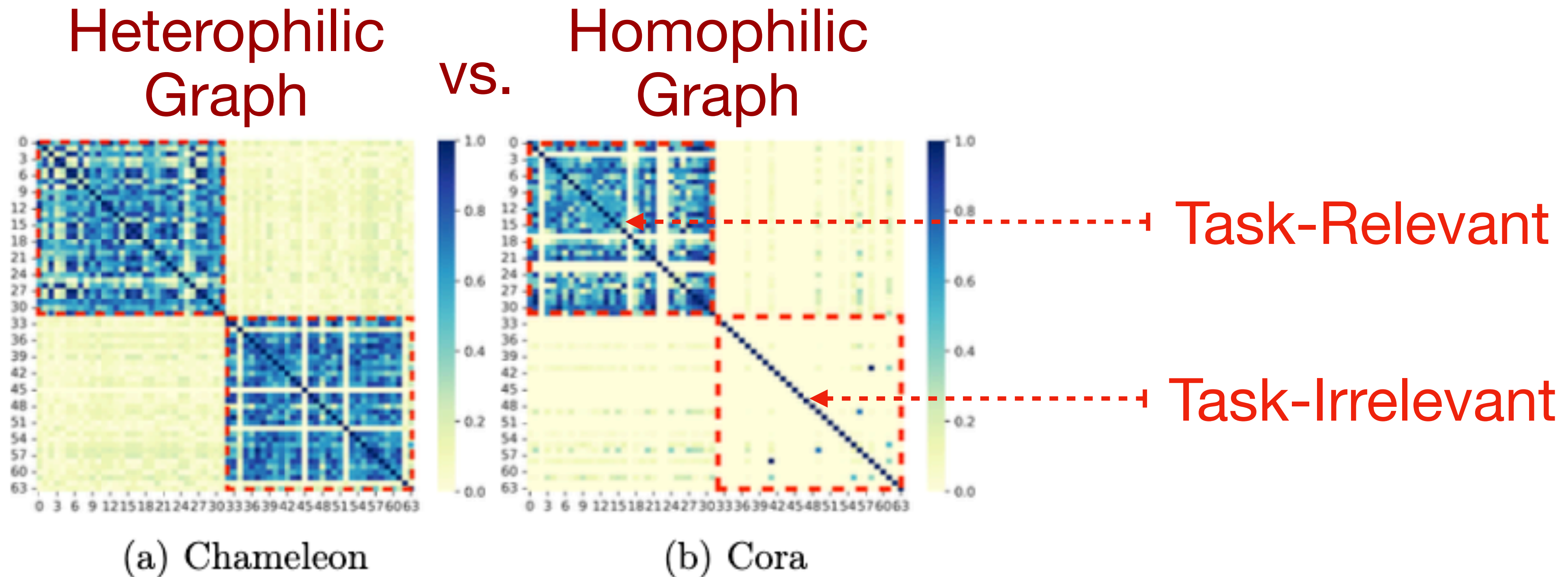
Two connected nodes share similarity in some features, **which could be either relevant or irrelevant (even harmful) to learning tasks**.



ES-GNN addresses heterophilic linking patterns by partitioning network topology and disentangling node features.

Proposed Works — Chapter 4: Edge Splitting GNN

Experimental Results

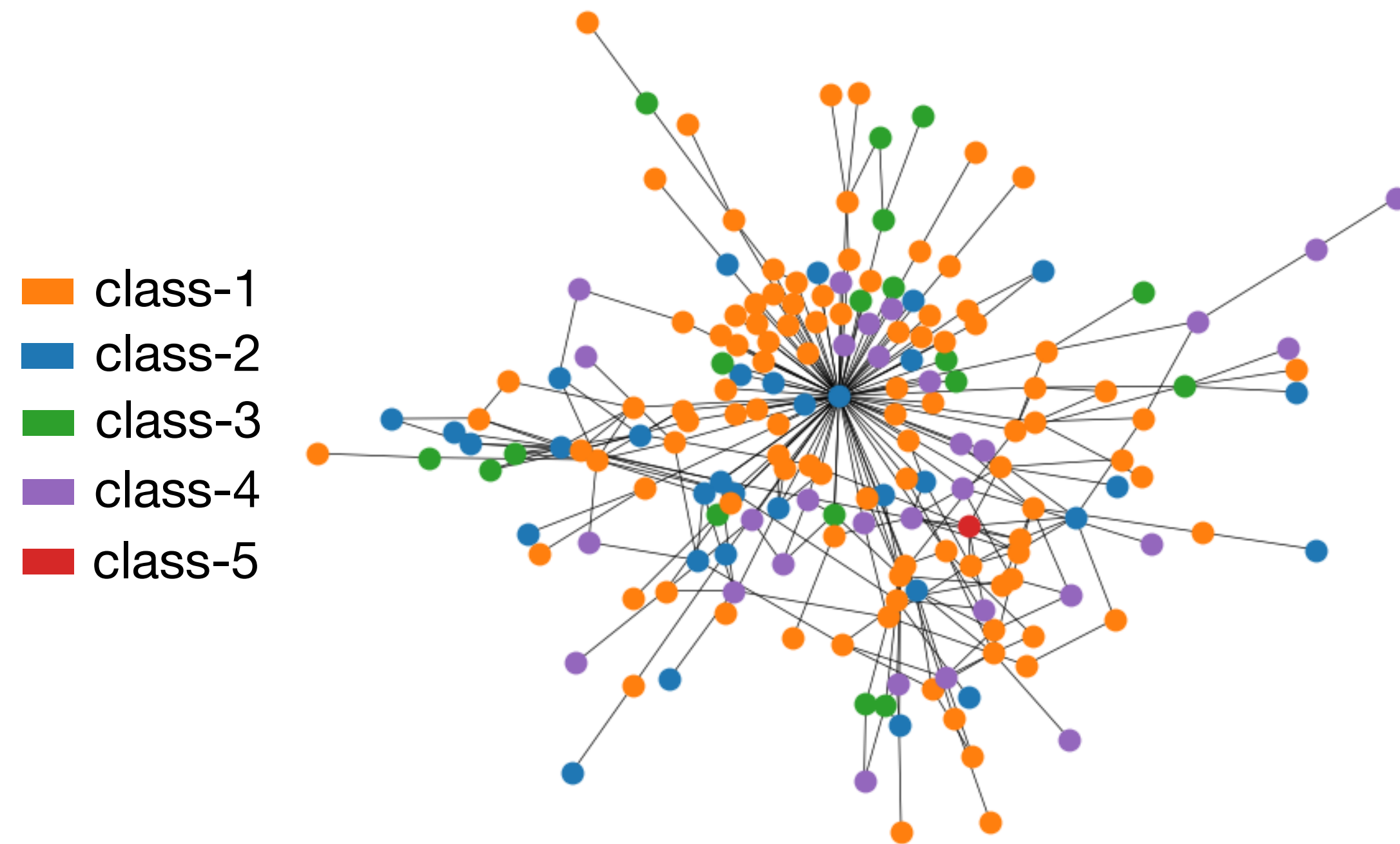


ES-GNN can disentangle task-relevant and irrelevant features, showcasing **universal adaptivity on different network types.**

Proposed Works — Chapter 5: Diverse Spectral Filtering

Linking Patterns in Heterophilic Graphs

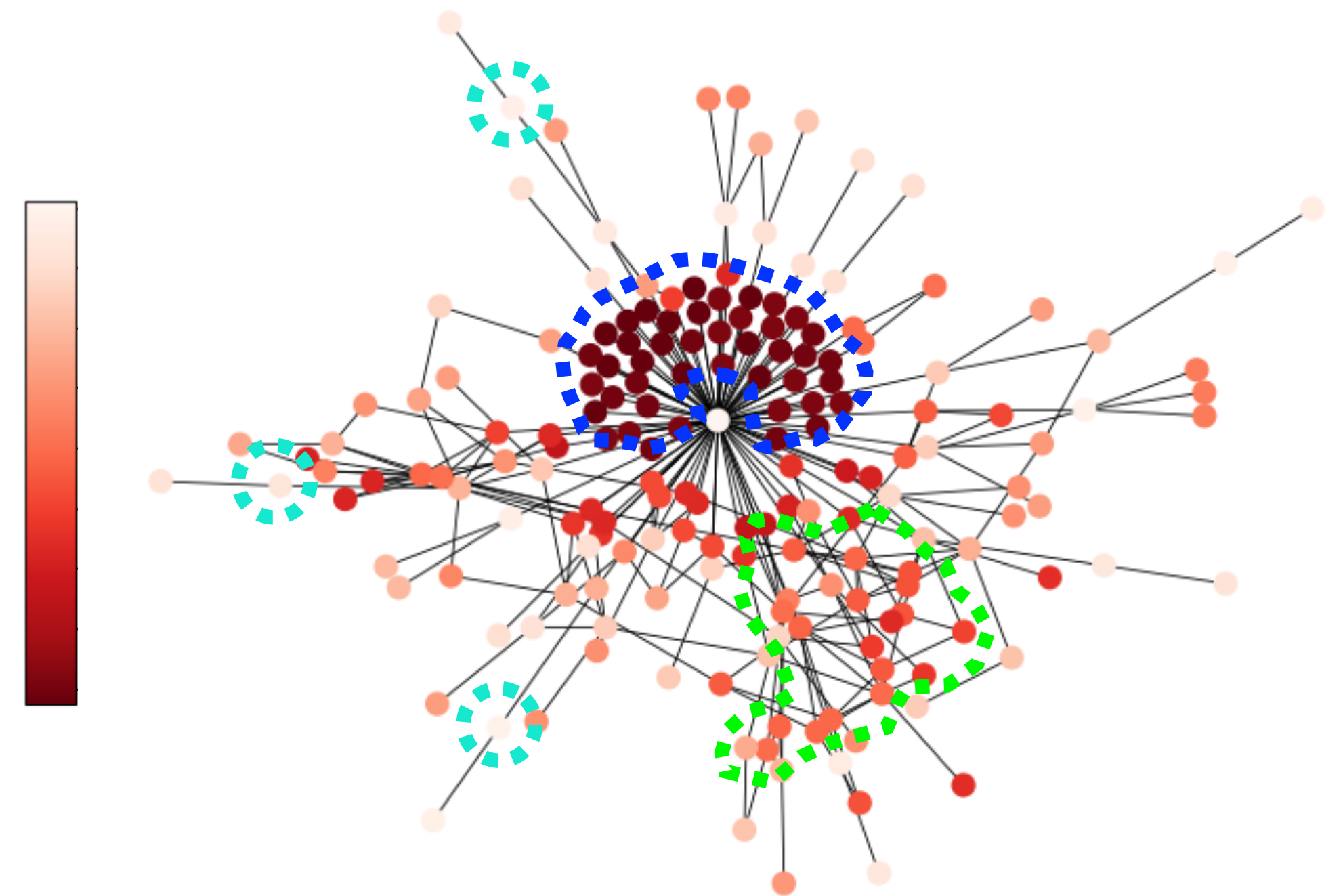
■ Edge-level (before)



most connected nodes are from different classes

Pairwise Heterogeneity

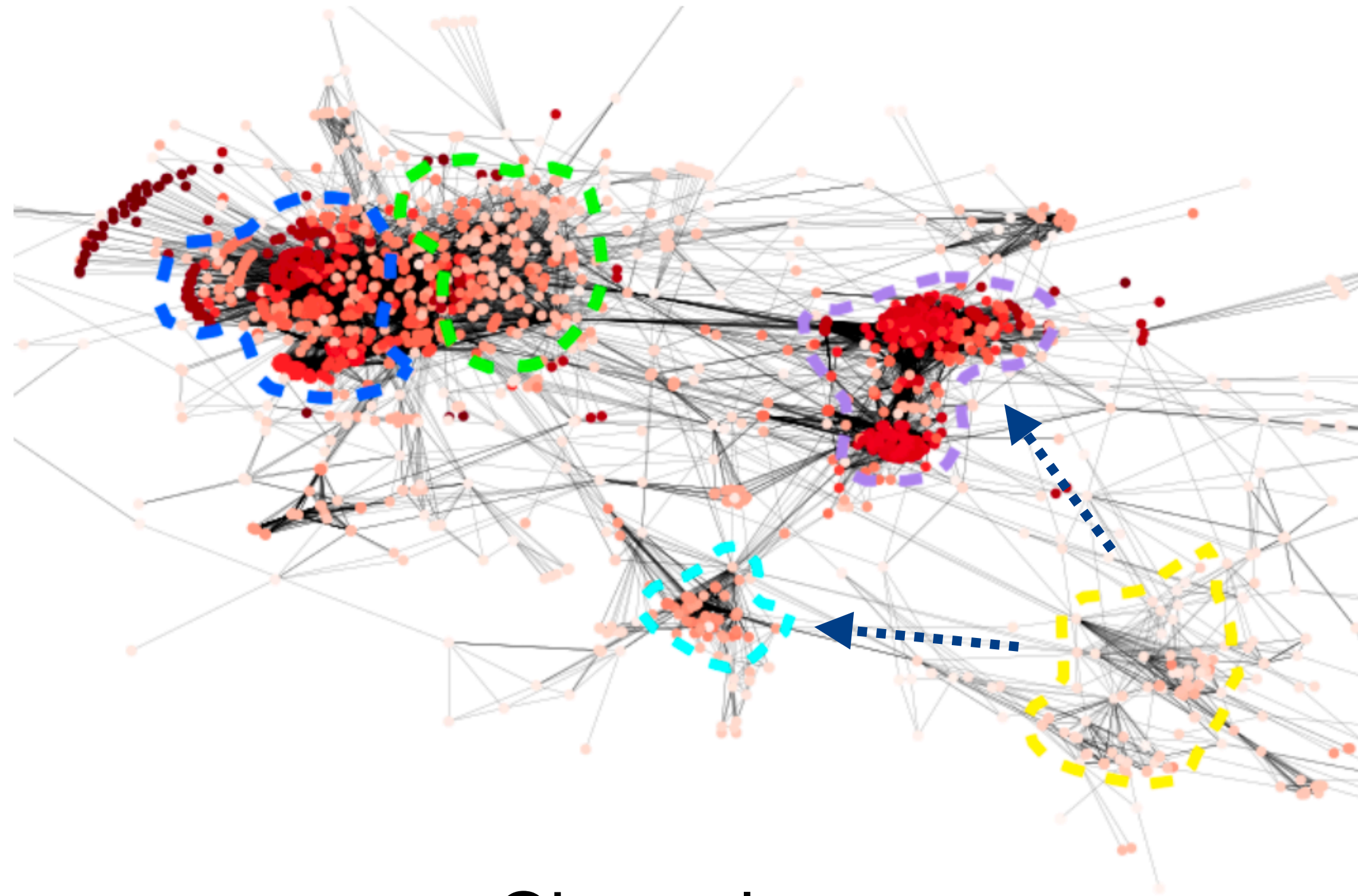
■ Subgraph-level (now)



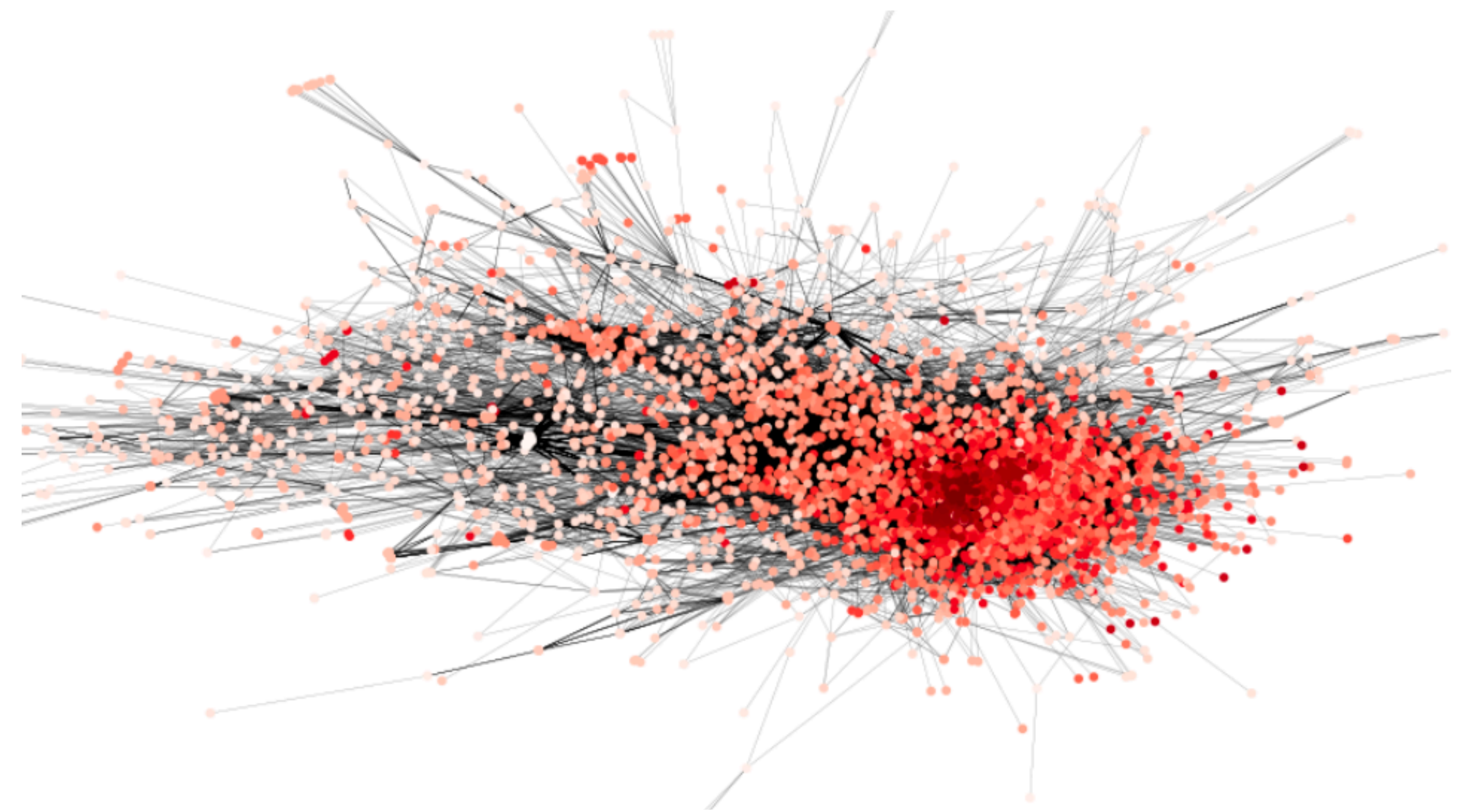
Regional Heterogeneity / Disparity

Proposed Works — Chapter 5: Diverse Spectral Filtering

Experimental Results



Chameleon



Squirrel

DSF can capture **regional disparity** with node-specific filter weights.

Jingwei Guo, et.al. Graph Neural Networks with Diverse Spectral Filtering. *WWW*, 2023.

Proposed Works — Chapter 6: Spatially Adaptive Filtering

■ Recall: Spectral GNNs

$$\mathbf{Z} = \mathbf{U}g_{\psi}(\Lambda)\mathbf{U}^T\mathbf{X} \quad \dashrightarrow \quad \text{theoretically rooted in spectral domain}$$

$$= g_{\psi}(\hat{\mathbf{L}})\mathbf{X} = \sum_{k=1}^K \psi_k P_k(\hat{\mathbf{L}})\mathbf{X} \quad \dashrightarrow \quad \text{practically relying on spatial approximation}$$

■ Spatial Interpretability?

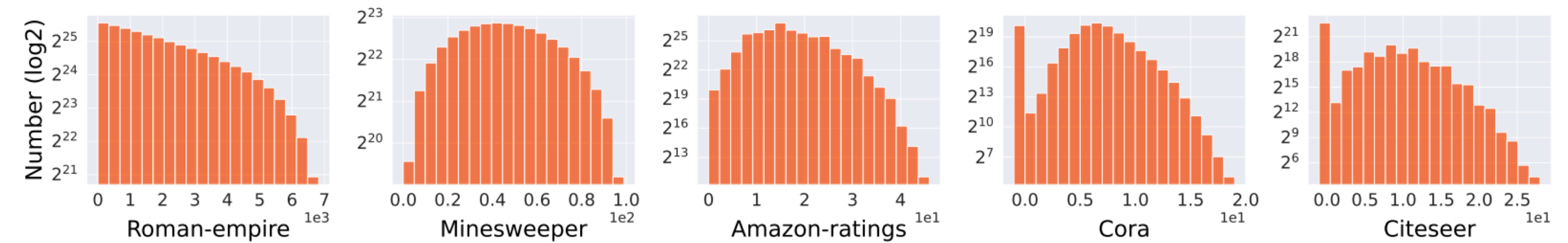


Figure 1: Distributions of connected nodes in the new graph based on their geodesic/shortest-path distance (as $\Delta_{i,j}$) in the original graph. Nodes, distant in the original graph ($\Delta_{i,j} > 1$ in x-axis), can be linked in the new graph (Number > 0 in y-axis).

$$\hat{\mathbf{A}}^{new} = \mathbf{I} - \frac{\alpha}{1 - \alpha} (g_{\psi}(\hat{\mathbf{L}})^{-1} - \mathbf{I})$$

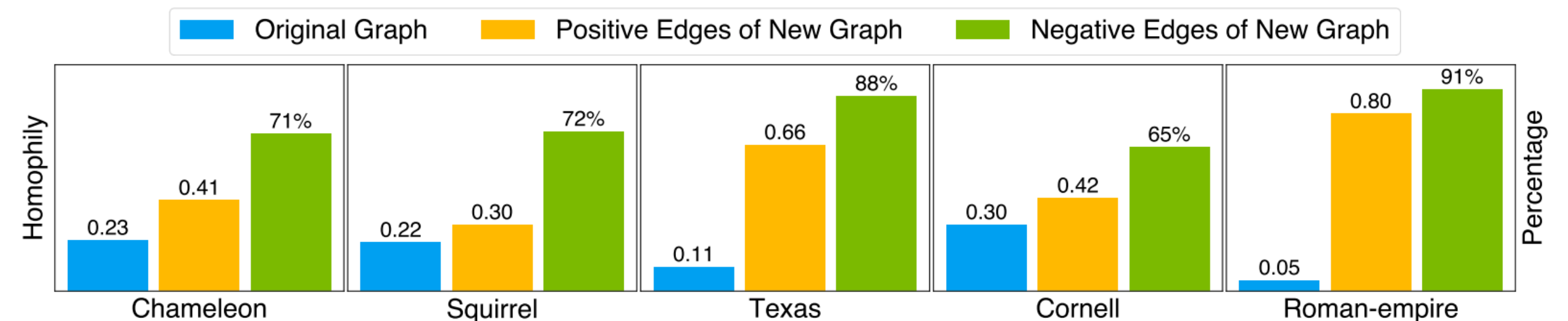
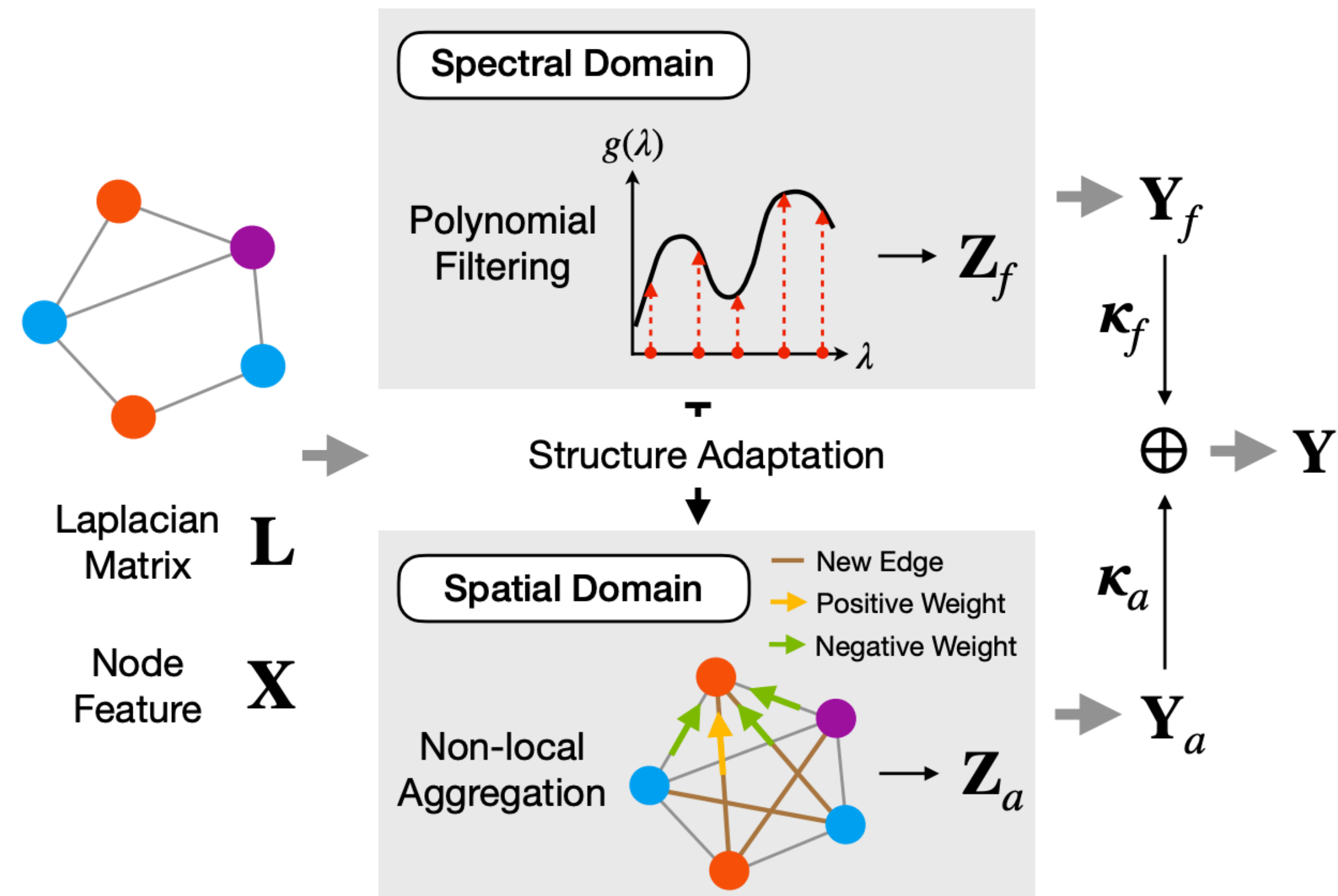


Figure 2: Left y-axis: Homophily comparison between original and new graphs, considering only positive edges (blue and yellow bars). Right y-axis: Percentage of edges connecting nodes from different classes, identified by negative edges (green bar).

Non-locality & Signed Edges

Proposed Works — Chapter 6: Spatially Adaptive Filtering

■ Ours: Spatially Adaptive Filtering



SAF leverages the adapted new graph by spectral filtering for **non-local aggregation with signed weights.**

Address:

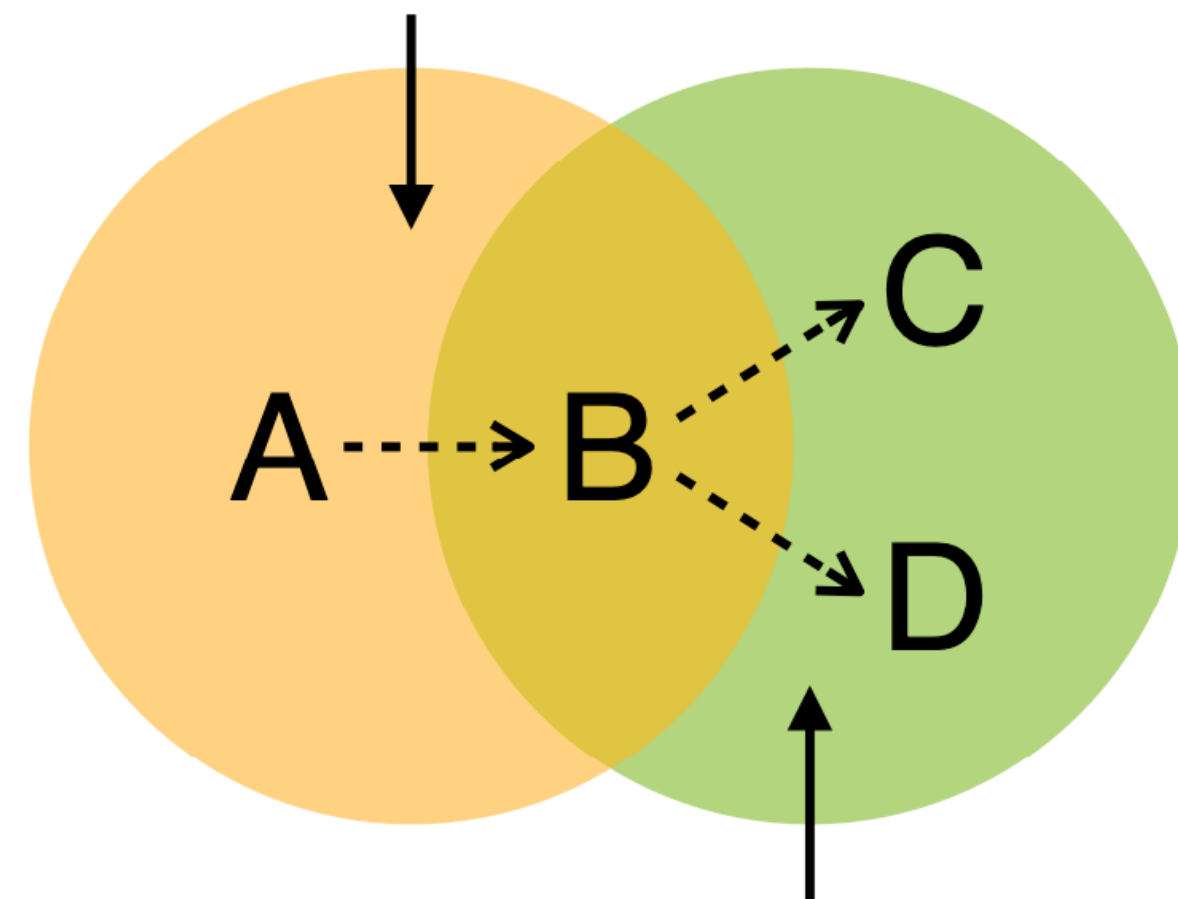
- Long-range Dependency
- Heterophilic Linking Patterns

Figure 3: Illustration of the proposed SAF framework, where varying node colors represent different node labels.

Conclusion — Research Aim

This thesis addresses the complex graph challenges of **Entangled Node Relationships** and **Heterophilic Linking Patterns** while learning GNNs across spatial and spectral domains.

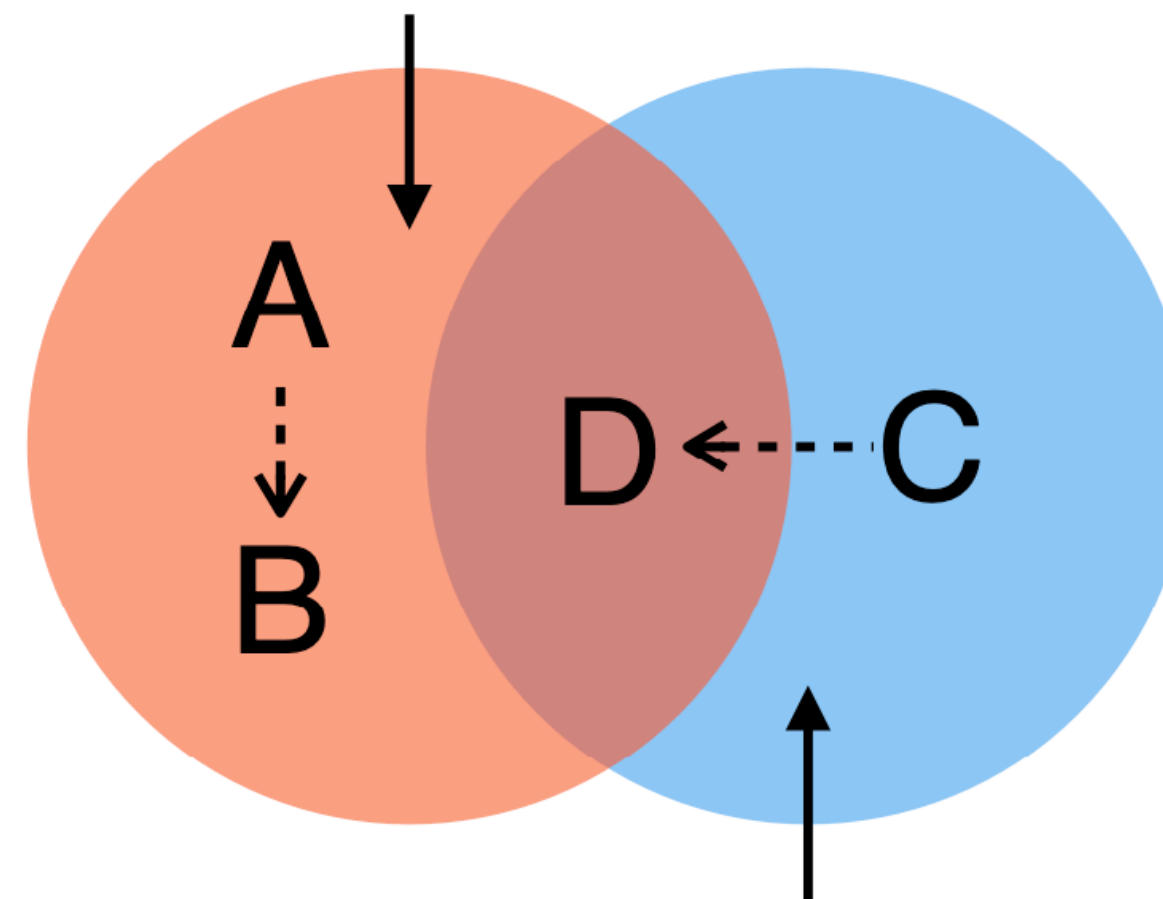
Entangled Node Relationships



Heterophilic Linking Patterns

Problem-Centric

Spatial Domain



Spectral Domain

Model-Centric

A: Chapter 3
B: Chapter 4
C: Chapter 5
D: Chapter 6

Conclusion — Research Outcome

■ Publications

Jingwei Guo, et.al. Graph Neural Networks with Diverse Spectral Filtering. *WWW, 2023*.

Jingwei Guo, et.al. Learning Disentangled Graph Convolutional Networks Locally and Globally. *TNNLS, 2022*.

■ Under review

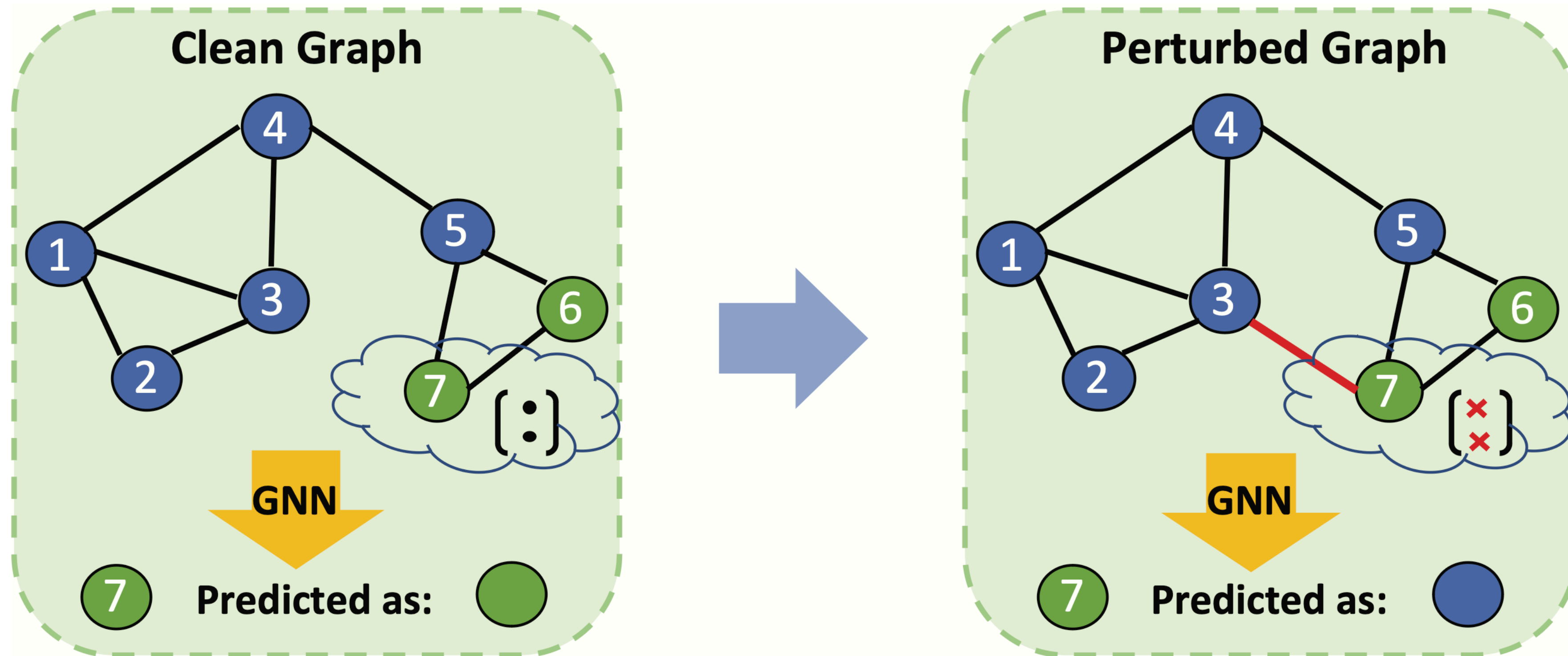
Jingwei Guo, et.al. ES-GNN: Generalizing Graph Neural Networks Beyond Homophily with Edge Splitting. *TPAMI, Under revision*.

Jingwei Guo, et.al. Rethinking Spectral Graph Neural Networks with Spatially Adaptive Filtering. *To be submitted*.

Future Work

▶ Graph Robustness

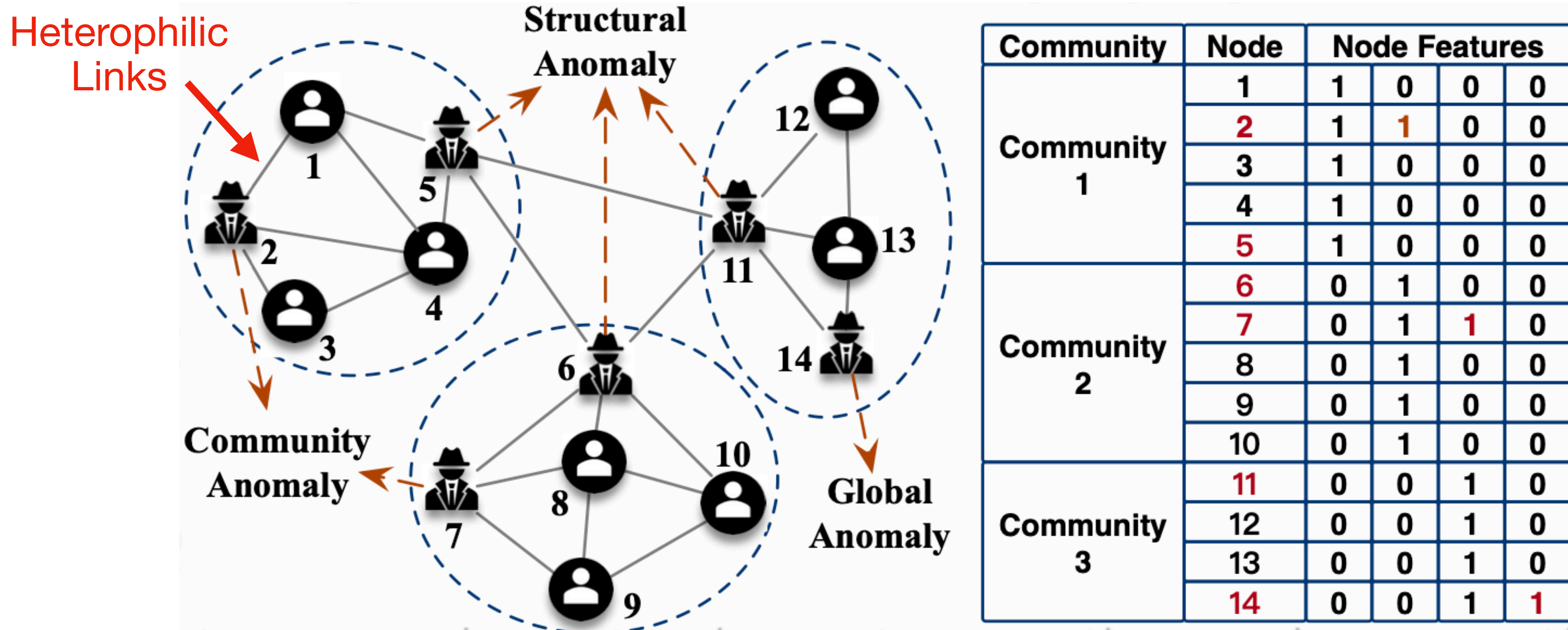
Homophilic Level ↓ / Heterophilic Level ↑



Enhancing GNN robustness by leveraging techniques from heterophilic graph learning.

Future Work

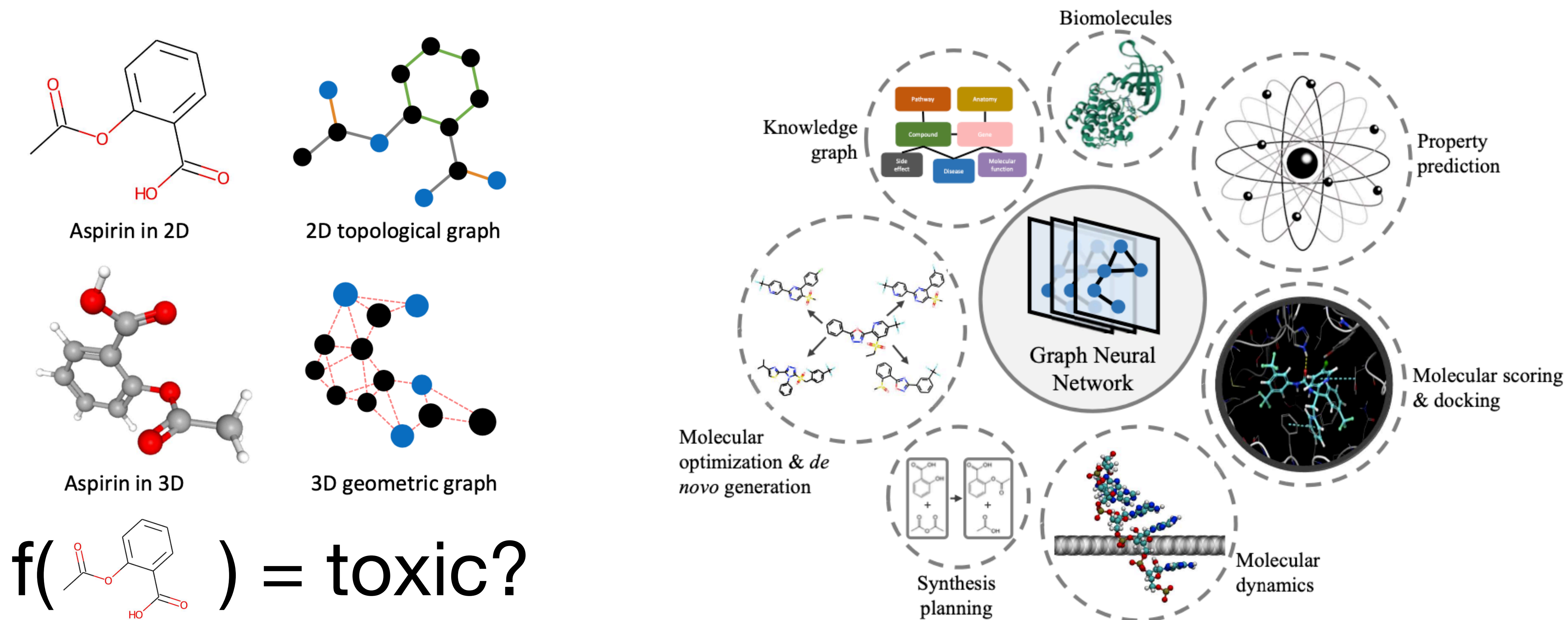
▶ Graph Anomaly Detection



GNNs can be used to detect scammers among benign users on transaction networks.

Future Work

► Molecular Science



GNNs are naturally suitable for modeling molecular systems.

Thanks!