

Multi-Component Coarsened Graph Learning for Scaling Graph Machine Learning

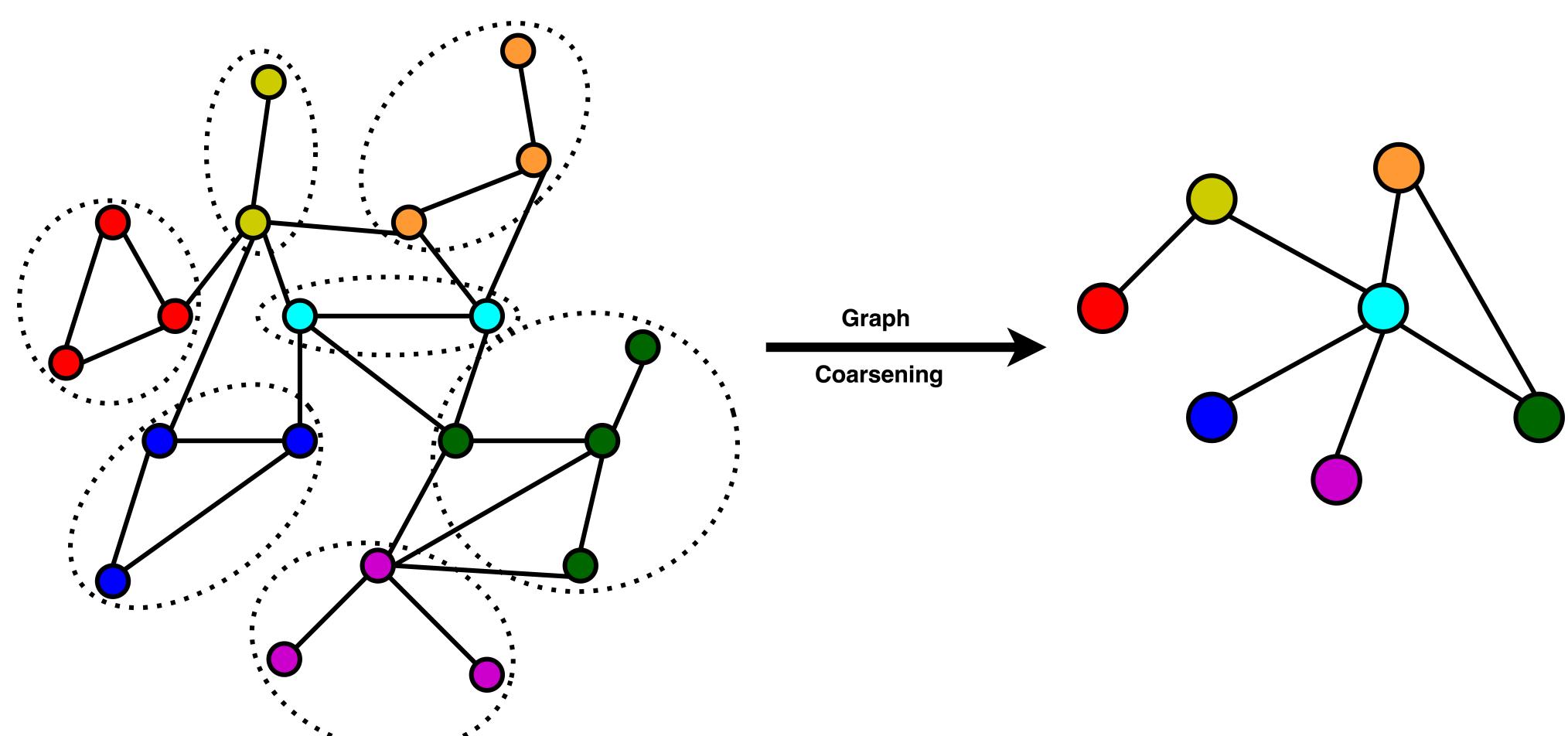


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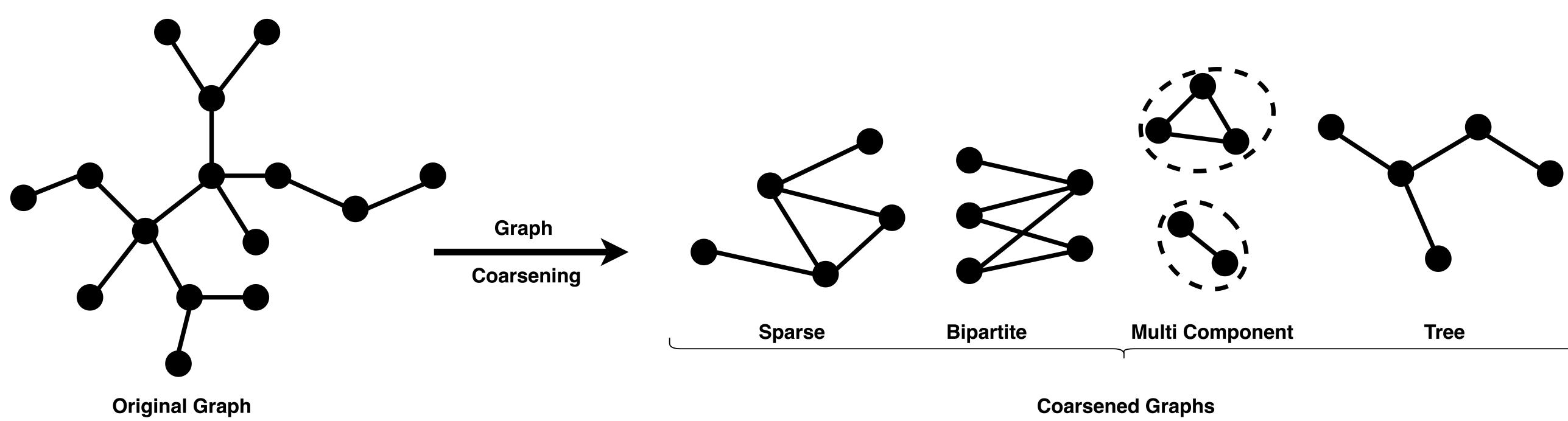
Graph Coarsening



- How do we map a large graph to a coarsened graph? Using $C \in \mathbb{R}_+^{p \times k}$, which belongs to $\mathcal{C} = \left\{ \langle C_i, C_j \rangle = 0 \forall i \neq j, \langle C_i, C_i \rangle = d_i, \|C_i\|_0 \geq 1, \|[C^T]_i\|_0 = 1 \right\}$
- How do we find Laplacian and feature matrix of the coarsened graph?

$$\Theta_c = C^T \Theta C, \quad X_c = P X, \quad X = P^\dagger X_c = C X_c$$

Structured Graph Reduction



Structured Graph Learning via Laplacian Spectral Constraints

This formulation uses the Laplacian matrix spectral properties to learn the Multi-component graph. The eigenvalues of the Laplacian matrix for an n-component graph are expressed as:

$$\mathcal{S}_\lambda = \{\{\lambda_j = 0\}_{j=1}^n, c_1 \leq \lambda_{n+1} \leq \dots \leq \lambda_k \leq c_2\} \quad (1)$$

where $n \geq 1$ denotes the number of connected components in the learned coarsened graph, and $c_1, c_2 > 0$ are constants that depend on the number of edges and their weights.

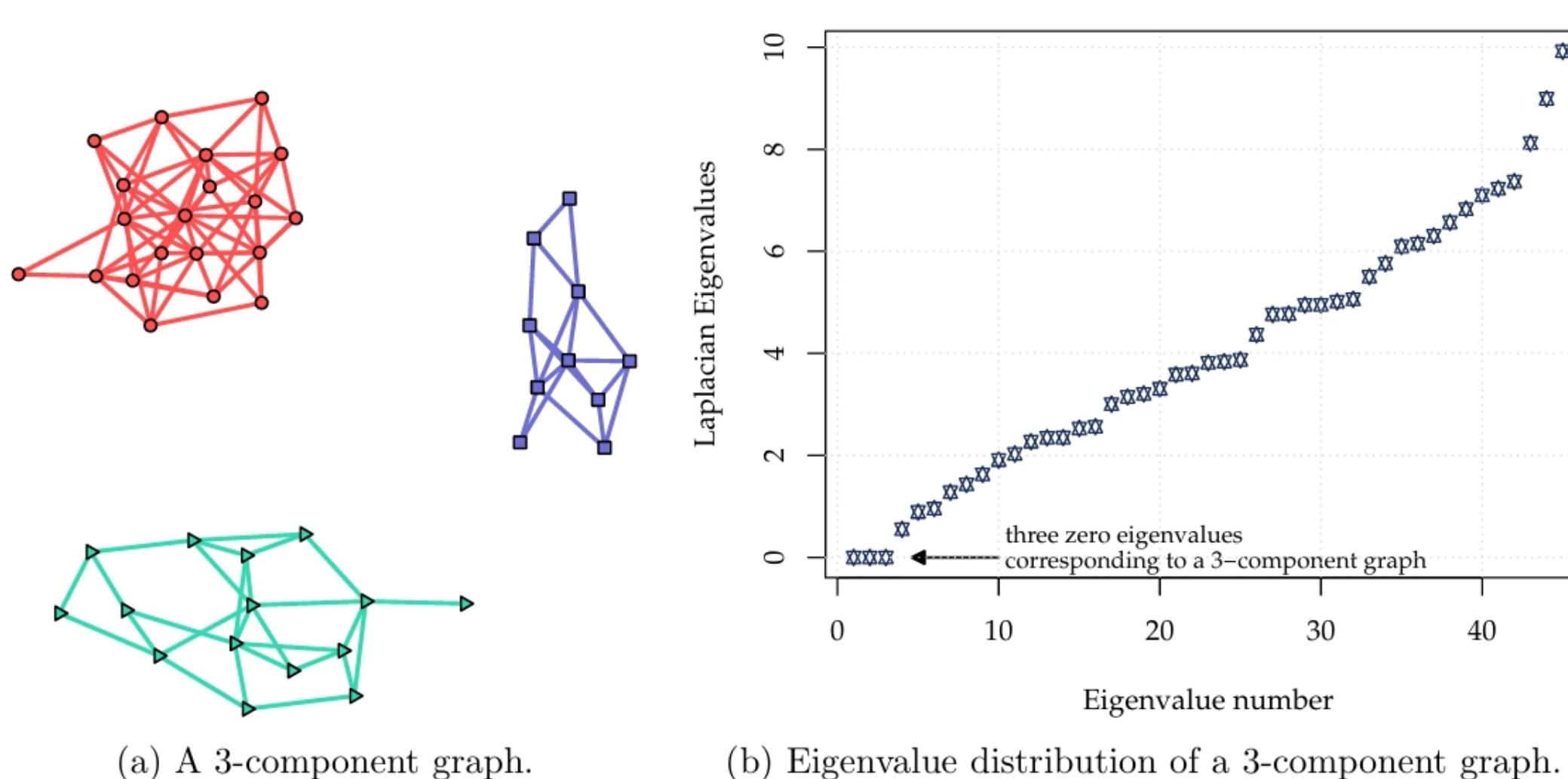


Figure 1. A 3-component graph and the eigenvalue distribution of its Laplacian matrix: three zero eigenvalues corresponding to three components.

Application of Multi-Component Graph

Recommendation	Edge Computing	Classification/Clustering
Capture diverse user-item interactions for improved recommendations.	Optimize dynamic application placement.	Accurately group nodes and classify graph entities.

Framework for Multi-Component Coarsened graph Learning

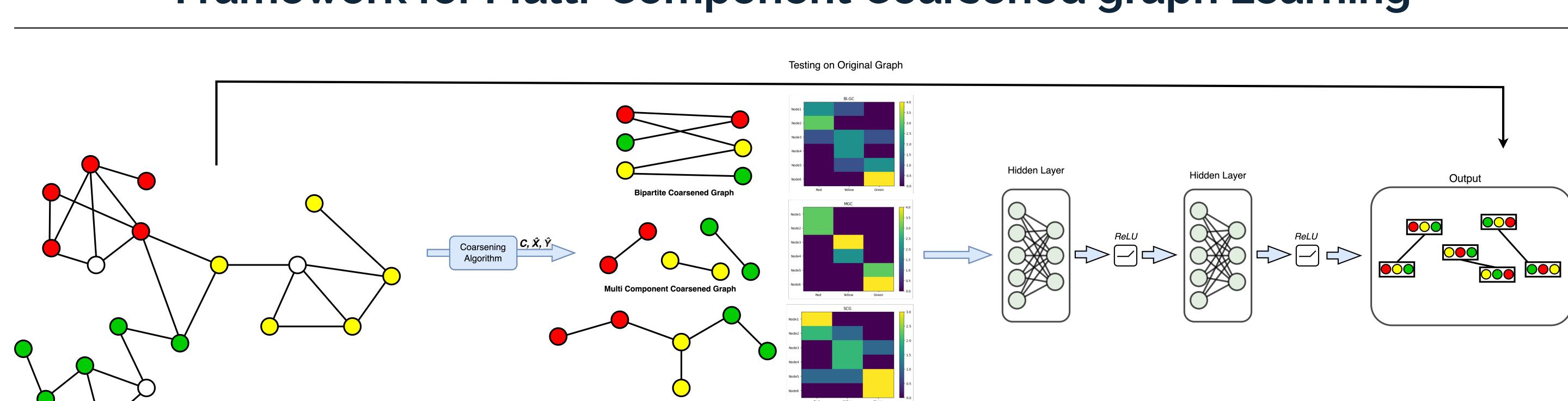


Figure 2. Sequence of steps in performing node classification task using a coarsened graph

Our approach for node classification using coarsened graph:

Input Graph: $G(A, X) \rightarrow$ Learn structured-coarsened graph $G_c(A_c, X_c, C)$ using $G(A, X) \rightarrow$ Label determination of coarsened graph $Y_c = \text{argmax}(C^T Y) \rightarrow$ Graph Neural Network training using $G_c(A_c, X_c, Y_c) \rightarrow$ Testing on Original graph

Optimization problem for MGC

$$\begin{aligned} \min_{C, \Lambda, U} & -\gamma \log \det(\Lambda) + \frac{\lambda}{2} \|C^T\|_{1,2}^2 + \frac{\beta}{2} \|C^T \Theta C - U \Lambda U^T\|_F^2 \\ \text{s.t. } & C \in \mathcal{S}_c = \left\{ C \geq 0 \mid \|[C^T]_i\|_2^2 \leq 1 \forall i = 1, \dots, p \right\}, \\ & U^T U = I, \quad \Lambda \in S_\lambda \end{aligned}$$

Algorithm

Proposed algorithm: Variables $\mathcal{X} = (\tilde{X}, C)$, solved using alternate block majorization-minimization:

$$\text{Sub-problem for } C : \min_{C \in \mathcal{S}_c} \frac{1}{2} C^T C - C^T A$$

$$\text{Sub-problem for } U : \min_{U^T U = I_q} \frac{\beta}{2} \|C^T \Theta C - U \Lambda U^T\|_F^2 = -\frac{\beta}{2} \text{tr}(U^T C^T \Theta C U \Lambda)$$

$$\text{Sub-problem for } \Lambda : \min_{\Lambda \in S_\lambda} -\gamma \log \det(\Lambda) + \frac{\beta}{2} \|C^T \Theta C - U \Lambda U^T\|_F^2$$

Algorithm 1: Multi-component Graph Coarsening (MGC)

- Input:** Graph Laplacian Θ , hyperparameters β, γ, λ
- while** stopping criteria not met **do**
- Update C:**
Compute gradient:
 $\nabla f(C^{(t)}) = \lambda C^{(t)} \mathbf{1} + 2\beta \Theta C^{(t)} (C^{(t)T} \Theta C^{(t)} - U \Lambda U^T)$
Update: $C^{(t+1)} = (C^{(t)} - \frac{1}{L} \nabla f(C^{(t)}))^\perp$
- Update U:**
 $U^{(t+1)}$ = eigenvectors of $C^T \Theta C$ corresponding to eigenvalues λ_{n+1} to λ_k
- Update Λ :**
Compute $d_i = (U^T C^T \Theta C U)_{ii}$ for $i = 1, \dots, q$
Update: $\lambda_i = \frac{1}{2}(d_i + \sqrt{d_i^2 + \frac{4\gamma}{\beta}})$
- end while**
- Return:** Final coarsening matrix C and coarsened Laplacian $\Theta_c = C^T \Theta C$

The worst-case computational complexity $O(p^2k)$

Node classification Using MGC

Data set	r=k/p	Baseline		Proposed
		GCOND	SCAL	MGC
CORA	0.5	81.02 ± 0.37	82.7 ± 0.50	87.20 ± 0.43
	0.3	81.56 ± 0.62	79.42 ± 1.71	84.56 ± 1.40
	0.1	79.47 ± 0.45	71.38 ± 3.62	76.02 ± 0.93
CITESEER	0.5	74.28 ± 1.45	72.04 ± 0.54	78.80 ± 1.20
	0.3	72.43 ± 0.94	68.87 ± 1.37	74.60 ± 2.31
	0.1	70.46 ± 0.41	68.58 ± 2.32	70.57 ± 1.25
PUBMED	0.1	78.57 ± 0.24	73.59 ± 3.56	84.81 ± 1.56
	0.05	78.16 ± 0.30	72.82 ± 2.62	81.89 ± 0.00
	0.03	78.04 ± 0.47	70.24 ± 2.63	80.70 ± 0.00
CO PHY	0.1	92.98 ± 0.52	86.43 ± 2.40	94.71 ± 0.22
	0.05	93.05 ± 0.26	73.09 ± 7.41	94.52 ± 0.19
	0.03	92.81 ± 0.31	63.65 ± 9.65	93.64 ± 0.25
NELL	0.1	77.3 ± 0.4	OOM	84.62 ± 0.85
OGBN-arxiv	0.1	61.3 ± 0.5	OOM	64.80 ± 1.90

Figure 3. Node classification accuracy on real datasets comparing the proposed MGC algorithms against GCOND and SCAL. MGC outperforms state-of-the-art methods across all datasets.

Comparison with Full dataset and Runtime Efficiency

Data set	MGC	Whole dataset
CORA	87.20 ± 0.43	89.51 ± 1.23
CITESEER	78.80 ± 1.20	78.09 ± 1.96
PUBMED	84.81 ± 1.56	88.89 ± 0.59

Figure 4. Node classification accuracy: GNN trained on the original graph (whole dataset) vs. the coarsened graph using MGC. Coarsened graph achieves similar accuracy with improved efficiency. OOM = Out Of Memory.

Dataset(r)	r = k/p	GCOND	SCAL	MGC	Whole dataset
CORA	0.05	329.86	27.76	2.78	2.86
CITESEER	0.05	331.33	56.21	3.73	5.24
PUBMED	0.05	202.04	54.09	46.09	58.85
CO-CS	0.05	1600.32	180.16	49.80	72.31

Figure 5. Computation time (τ): Time (in sec.) for coarsening and node classification with a ratio of 0.05. MGC is faster than SOTA baselines and even faster than classification on the full graph.

References

- [SBP17] Y. Sun, P. Babu, and D. P. Palomar. Majorization-Minimization Algorithms in Signal Processing, Communications, and Machine Learning. ()
- [JLJ20] Y. Jin, A. Loukas, and J. Jaja. Graph Coarsening with Preserved Spectral Properties.
- [Kum+20] S. Kumar et al. A unified framework for structured graph learning via spectral constraints. ()
- [Jin+21] W. Jin et al. Graph Condensation for Graph Neural Networks. arXiv: 2110.07580 [cs.LG].
- [Kum+23] M. Kumar et al. Featured Graph Coarsening with Similarity Guarantees.