# Towards Optimal Graph Compression: Learning Coarsened Graphs with Desirable Properties for Practical Applications

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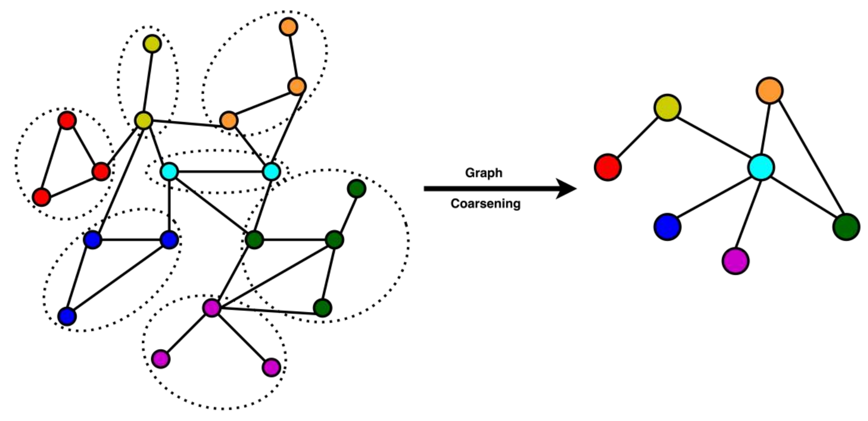
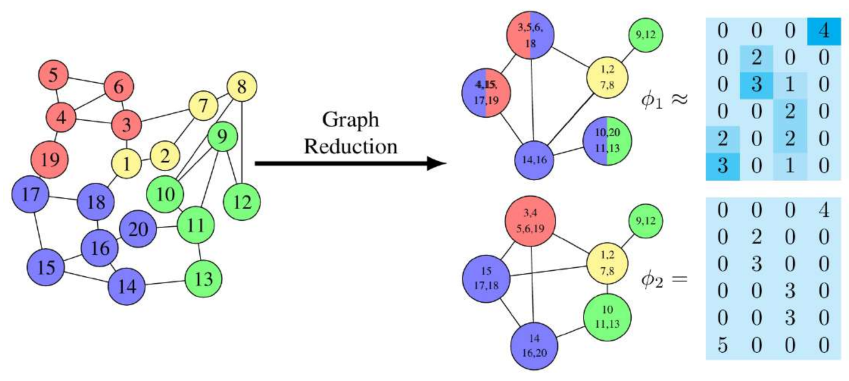
## Graph Coarsening




- How do we map a large graph to a coarsened graph? Using $C \in \mathbb{R}_+^{p\times k}$, which belongs to
$$\mathcal{C} = \Big\{ \langle C_i, C_j\rangle = 0 \;\forall\, i \neq j,\quad \langle C_i, C_i\rangle = d_i, \|C_i\|_0 \geq 1, \|[C^T]_i\|_0 = 1 \Big\}$$
- How do we find Laplcaian and feature matrix of the coarsened graph?
$$\Theta_c = C^T\Theta C, \quad X_c = PX, \quad X = P^{\dagger}X_c = CX_c$$

## Quality of Coarsened Graph




- Node Profile Matrix : $\phi = C^TY$ ; $Y \in \mathbb{R}_+^{p\times l}$ represents one-hot label matrix of the original graph.

A loading matrix $C$ is considered balanced, and a coarsened graph is considered informative when, after transforming the one-hot matrix $Y \in \mathbb{R}^{p\times l}$ of labels from the original graph $\mathcal{G}$ using $C$, the resulting matrix $\phi = C^TY$ exhibits sparsity in its rows.

## Research objectives

The present study investigates the following objectives:

- **Objective 1:** Optimization Framework for Semi-supervised Attributed Graph Coarsening (Accepted in UAI'24)
- **Objective 2:**Structured Graph Reduction for Efficient GNN (Accepted in WWW'25)
- **Objective 3:**Coarse-and-learn: Efficient Entropy based Coarsening and online node labeling
- **Objective 4:**Graph based Coarse-graining Molecular dynamics with Force Matching

## Optimization Framework for Semi-supervised Attributed Graph Coarsening

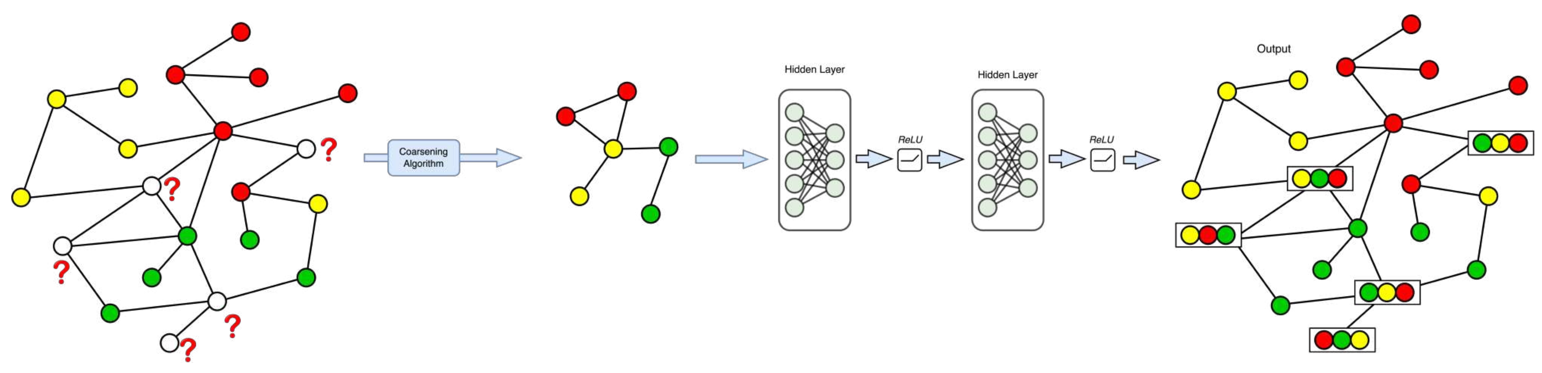



Figure 1. Sequence of steps in performing node classification task using a coarsened graph

Existing state of the art work flow for node classification using coarsened graph:

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

Our approach for node classification using coarsened graph:

Input Graph: $G(A, X, Y)$ $\rightarrow$ Learn coarsened graph $G_c(A_c, X_c, Y_c)$ using $G(A, X, Y)$ $\rightarrow$ Graph Neural Network training using $G_c(A_c, X_c, Y_c)$ $\rightarrow$ Testing on Original graph

## Optimization Problem for LAGC

$$\min_{\tilde{X}, C} -\gamma\log\det(C^T\Theta C + J) + \text{tr}(\tilde{X}^TC^T\Theta C\tilde{X}) + ||C\tilde{X} - X||_F^2 + \frac{\lambda}{2}\|C^T\|_{1,2}^2 + \frac{\beta}{2}\|C^T\Theta C\|_F^2 + \frac{\delta}{2}\|C^TY\|_F^2$$
$$\text{s.t. } \mathcal{S}_C = \Big\{ C \geq 0 |\; \|[C^T]_i\|_2^2 \leq 1 \;\forall\, i = 1, .., p \Big\}$$

## Algorithm

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

$$\text{Sub-problem for } C: \quad \min_{C\in\mathcal{S}_c} \; \frac{1}{2}C^TC - C^TA$$
$$\text{Sub-problem for } \tilde{X}: \quad \min_{\tilde{X}} \text{tr}(\tilde{X}^TC^T\Theta C\tilde{X}) + \alpha 2\|C\tilde{X} - X\|_F^2$$

**The LAGC Algorithm summary**

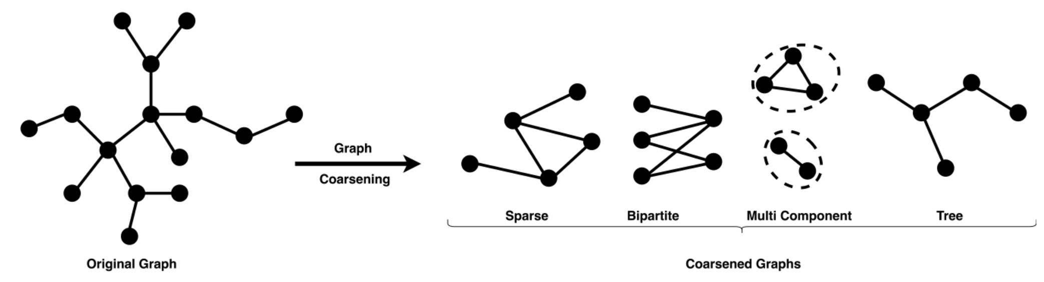
1: **Input:** $\mathcal{G}(X, \Theta), \alpha, \gamma, \lambda$.
2: **while** Stopping criteria not met **do**
3: $\quad C^{(t+1)} = \left(C^{(t)} - \frac{1}{L}\nabla f\left(C^{(t)}\right)\right)^+$
4: $\quad \tilde{X}^{t+1} = \left(\frac{2}{\alpha}C^T\Theta C + C^TC\right)^{-1}C^TX$
5: **end while**
6: Return $C^{t+1}$, $\tilde{X}^{t+1}$

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

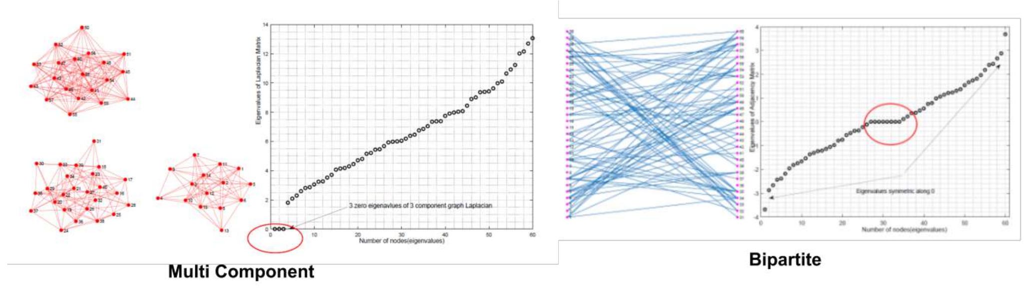
## Node classification Using LAGC

| Data set | r=k/p | GCOND | SCAL | FGC | LAGC | Whole Data |
|---|---|---|---|---|---|---|
| CORA | 0.3 | 81.56 ± 0.62 | 79.42 ± 1.71 | 84.03 ± 0.08 | **87.62 ± 0.01** | 89.50 ± 1.20 |
| | 0.1 | 81.37 ± 0.40 | 71.38 ± 3.62 | 79.96 ± 0.18 | **86.10 ± 0.03** | |
| | 0.05 | 78.93 ± 0.44 | 55.32 ± 7.03 | 77.31 ± 0.65 | **82.85 ± 0.02** | |
| CITESEER | 0.3 | 72.43 ± 0.49 | 68.87 ± 1.37 | 72.85 ± 0.10 | **78.51 ± 1.25** | 78.09 ± 1.95 |
| | 0.1 | 70.46 ± 0.49 | 71.38 ± 3.62 | 69.46 ± 0.22 | **76.00 ± 0.50** | |
| | 0.05 | 64.03 ± 2.40 | 55.32 ± 7.03 | 69.02 ± 0.24 | **75.70 ± 0.31** | |
| CO-PHYSICS | 0.05 | 93.05 ± 0.26 | 73.09 ± 7.41 | 93.31 ± 0.11 | **94.46 ± 0.58** | 96.22 ± 0.74 |
| | 0.03 | 92.81 ± 0.31 | 63.65 ± 9.65 | 92.00 ± 1.78 | **94.28 ± 0.21** | |
| | 0.01 | 92.81 ± 0.31 | 63.65 ± 9.65 | 91.08 ± 0.78 | **93.26 ± 0.89** | |
| PubMed | 0.05 | 78.16 ± 0.30 | 72.82 ± 2.62 | 78.14 ± 0.29 | **82.85 ± 0.32** | 88.89 ± 0.57 |
| | 0.03 | 78.04 ± 0.47 | 70.24 ± 2.63 | 77.60 ± 0.16 | **82.10 ± 0.21** | |
| | 0.01 | 77.20 ± 0.02 | 50.49 ± 10.5 | 76.10 ± 1.91 | **81.27 ± 0.91** | |
| CO-CS | 0.05 | 86.29 ± 0.63 | 34.45 ± 10.0 | 89.12 ± 0.08 | **91.36 ± 0.48** | 93.32 ± 0.62 |
| | 0.03 | 86.32 ± 0.45 | 26.06 ± 9.29 | 86.32 ± 0.43 | **90.32 ± 0.97** | |
| | 0.01 | 84.01 ± 0.02 | 14.42 ± 8.51 | 85.41 ± 0.24 | **88.27 ± 0.34** | |
| DBLP | 0.05 | 79.15 ± 0.20 | 76.52 ± 2.88 | 80.08 ± 0.01 | **81.64± 0.42** | 85.35± 0.86 |
| | 0.03 | 78.42 ± 1.26 | 75.49 ± 2.84 | 79.92 ± 0.48 | **80.93± 0.12** | |
| | 0.01 | 74.29 ± 0.57 | 72.01± 1.83 | 77.47 ± 0.33 | **79.49 ± 0.53** | |

## Structured Graph Reduction for Efficient GNN




Structured Graph using Spectral Constraint




- Multi-component Coarsened graph:
$$\lambda(\mathcal{T}(\Theta_c^s)) \in \mathcal{S}_\lambda = \Big\{ \{\lambda_j = 0\}_{j=1}^n, c_1 \leq \lambda_{n+1} \leq \ldots \leq \lambda_k \leq c_2 \Big\}$$
- Bi-partite Coarsened graph Graph:

## Online coarse-and-learn for Large Graphs

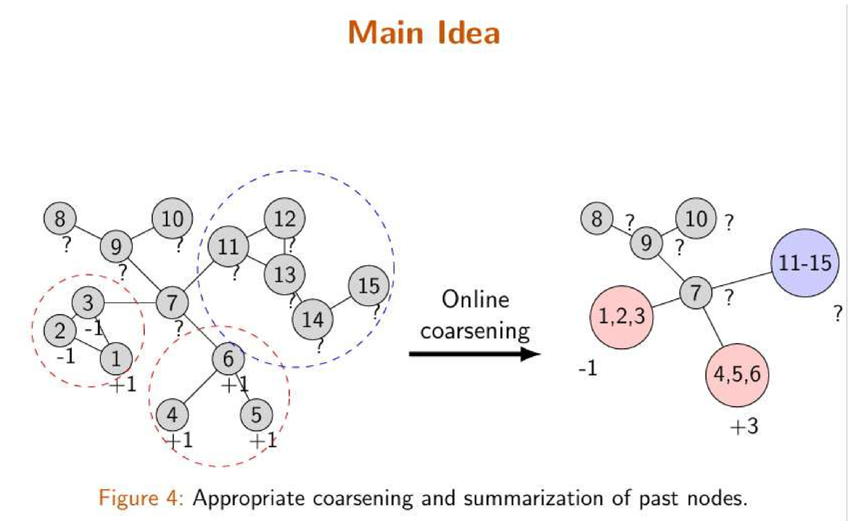



Figure 2. Appropriate coarsening and summarization of past nodes.

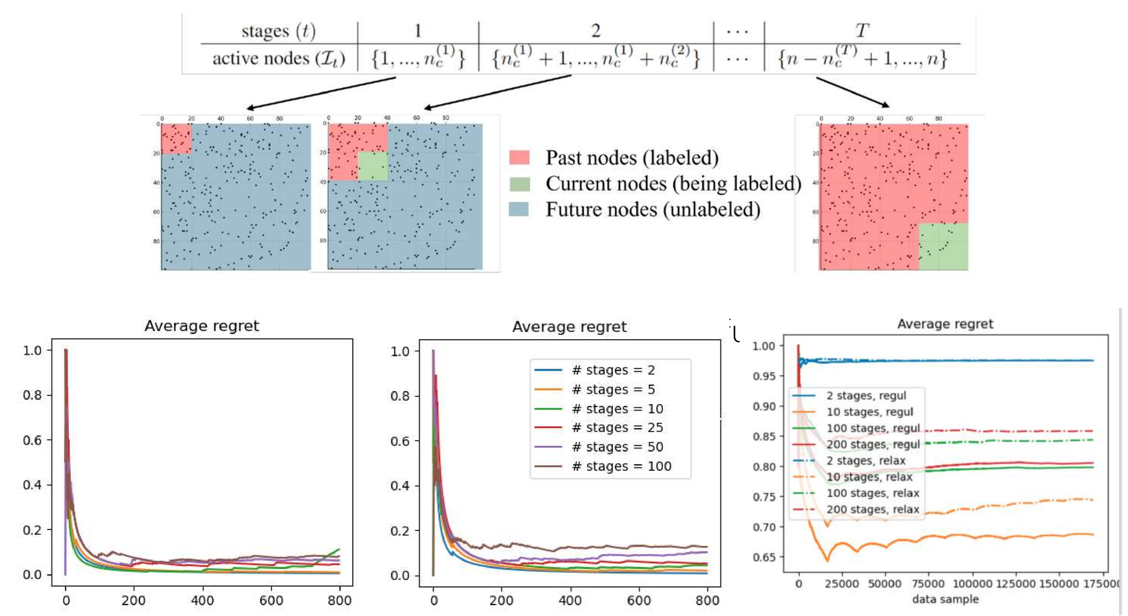
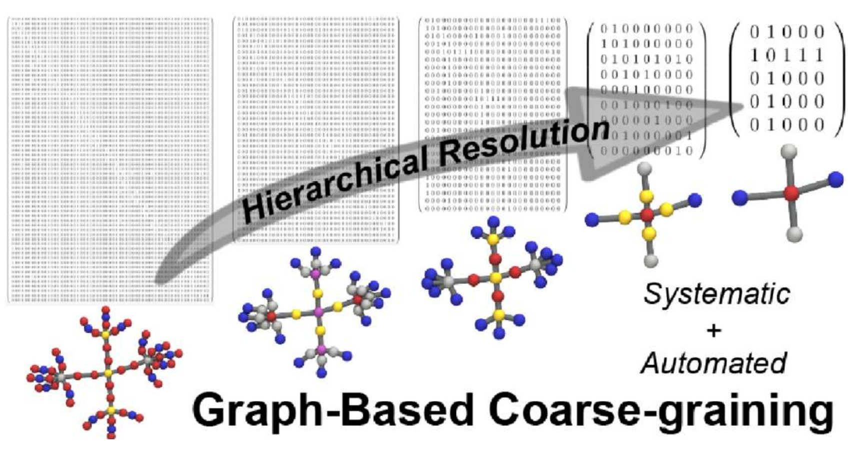



Figure 4. Average regret for experiment A (left) and B (center). Right: Average regret for ogbn-arxiv (1.15 million nodes).

## Graph based Coarse-graining Molecular dynamics with Force Matching




## References

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## Subhanu's Portfolio Website