Graph Coarsening and Graph Neural Networks

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Joint work with **Antonin Joly** and **Aline Roumy**

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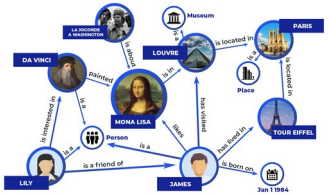
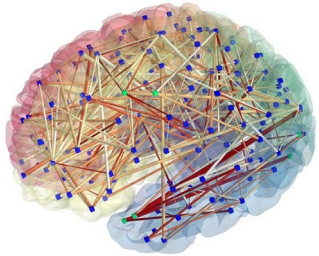
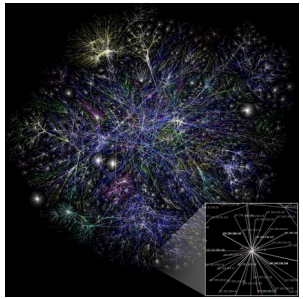
Why care about graphs?



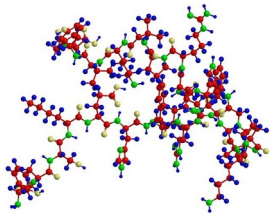
Knowledge graph



Brain connectivity network

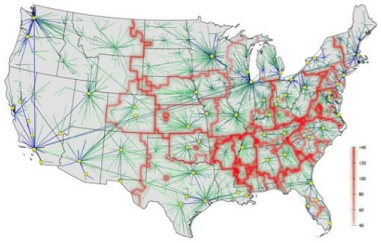


Internet



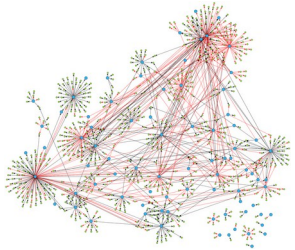
Molecule

Social network

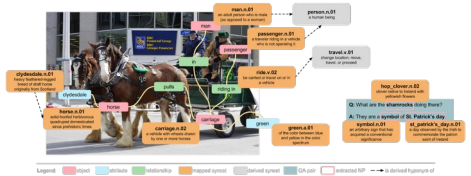


Transportation network

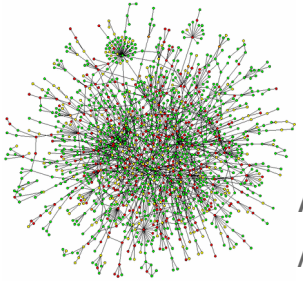
Computer network



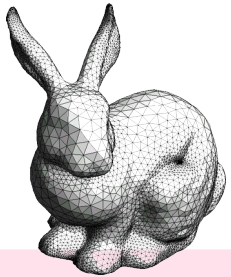
Gene regulatory network



Scene understanding network



Protein interaction network



3D mesh

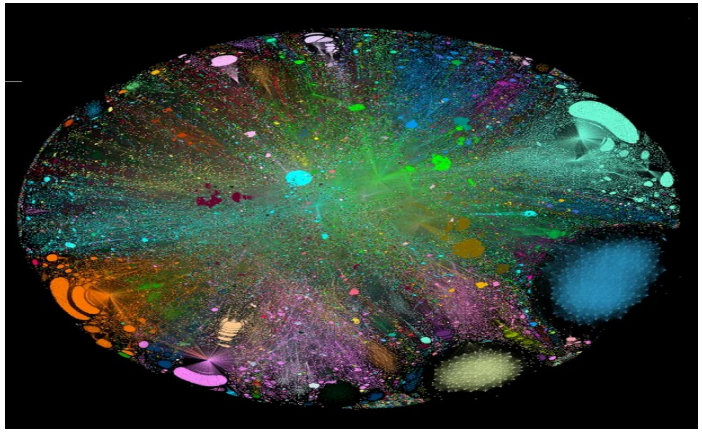
- **Many types of interesting data** can be represented as graphs

  "if all you have is a hammer, everything looks like a nail"

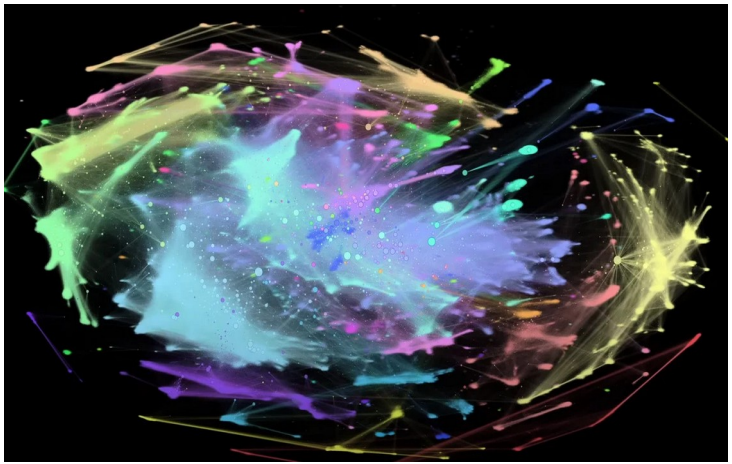
- Modern Graph ML is "part of/referred to as" **Geometric Deep Learning**

Large graphs

- Modern graphs are HUGE
- Any reasonable processing pipeline includes **graph reduction methods**



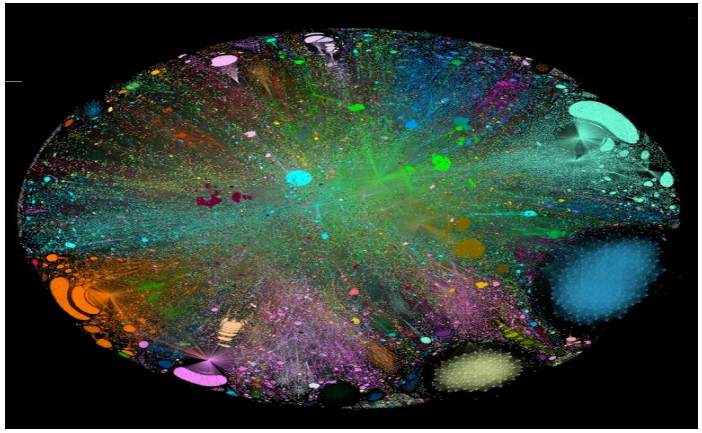
Reddit
200k nodes, 114M edges



Wikipedia
6M nodes, 200M edges

Large graphs

- Modern graphs are HUGE
- Any reasonable processing pipeline includes **graph reduction methods**
- **Two** main kinds:
  - Graph sampling
  - Graph coarsening



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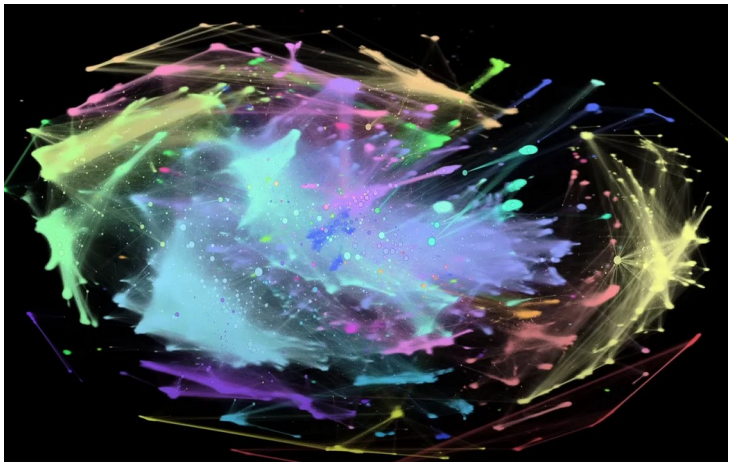

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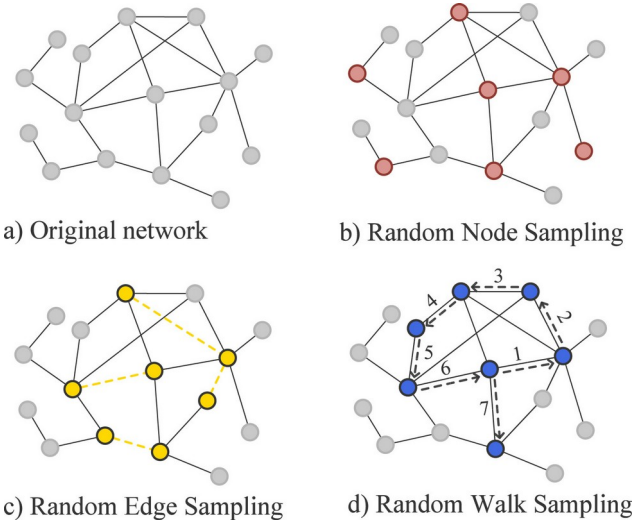
Graph sampling

- **Sample** nodes/edges from a large graph



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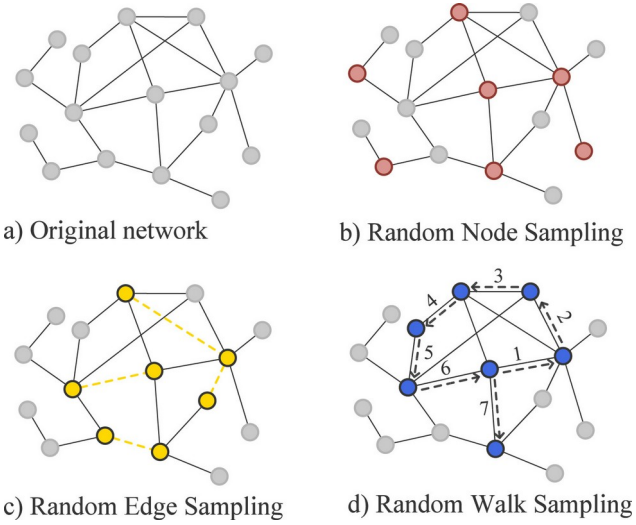
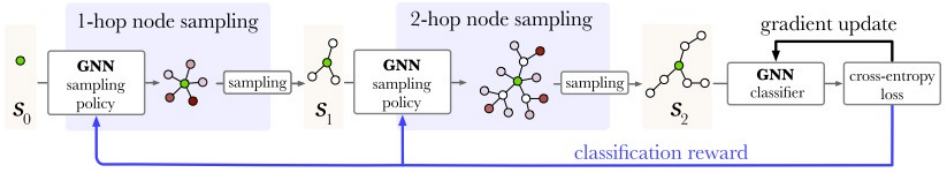
- **Pros**:
  - Light, fast
  - Can be done at many stages
  - Many different samplers





Graph sampling

- **Sample** nodes/edges from a large graph

- **Pros**:
  - Light, fast
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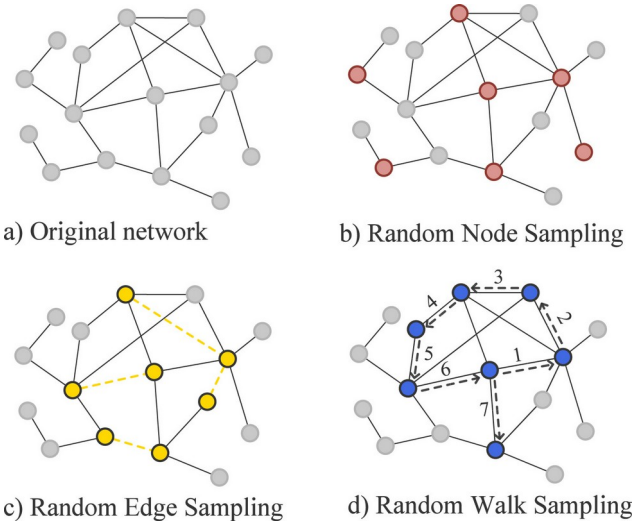
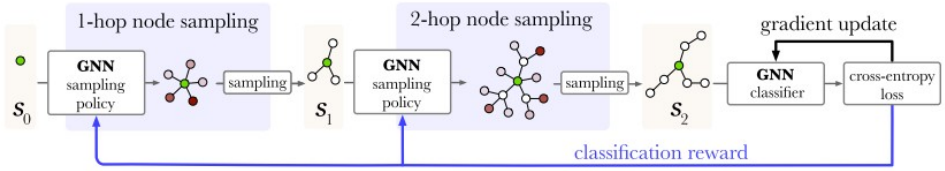
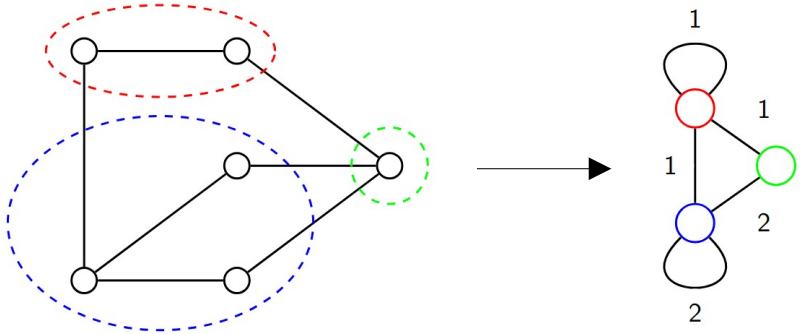
- **Cons**:
  - Extracting a subgraph
  - Difficult to control the loss of information
  - k-hop sampling vs. small-world graphs





Graph coarsening

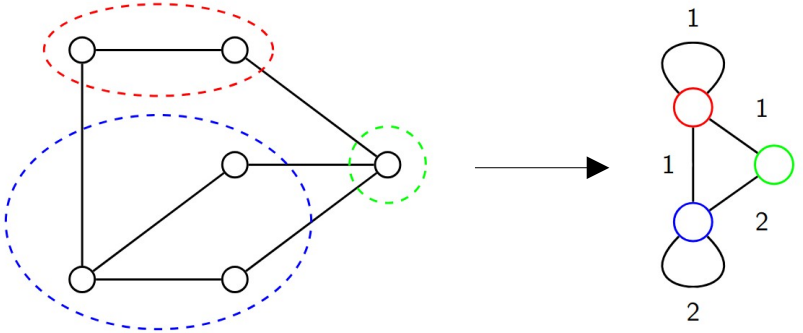
- **Create** a small graph from a large graph

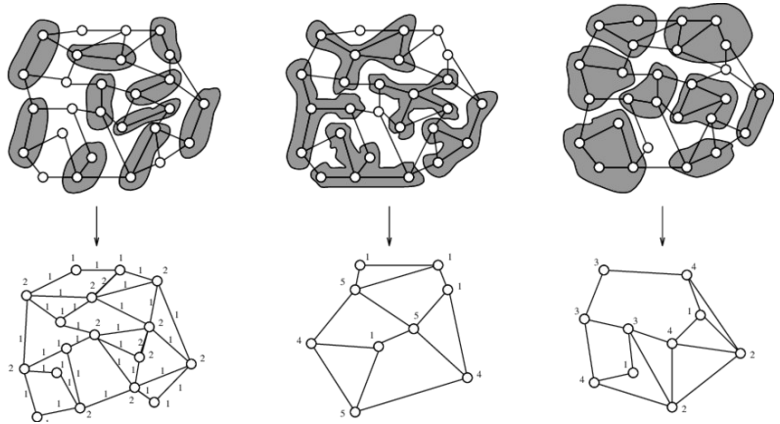


Graph coarsening

- **Create** a small graph from a large graph

- **Pros**:
  - Theoretically more consistent
  - Many algorithms
  - The small graph often already *means* something!





Different ways to coarsen a graph

Graph coarsening

- **Create** a small graph from a large graph
- **Pros**:
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  - Many algorithms
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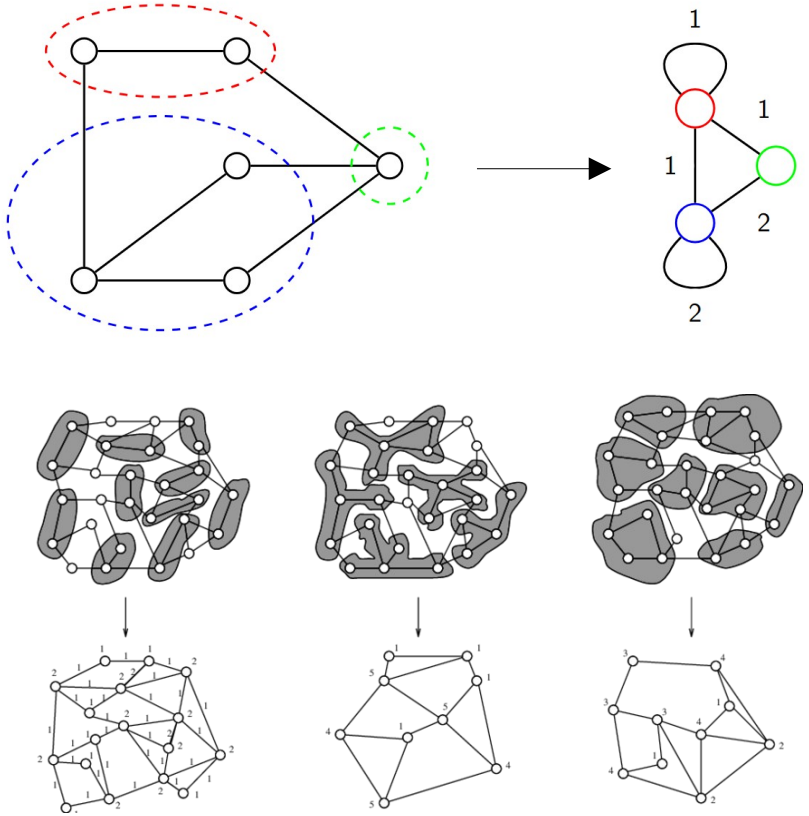
- **Cons**:
  - Graph "learning" is difficult
  - Computationally costly!



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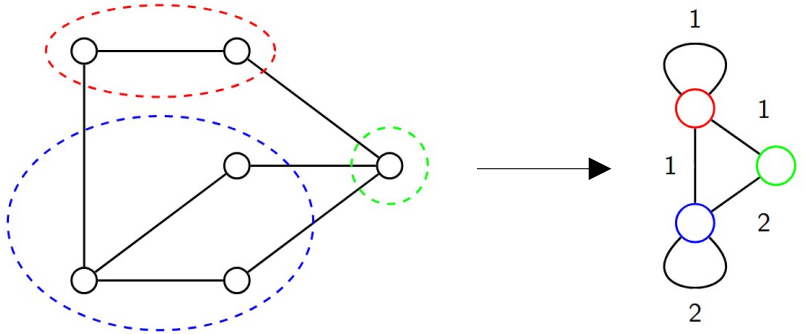

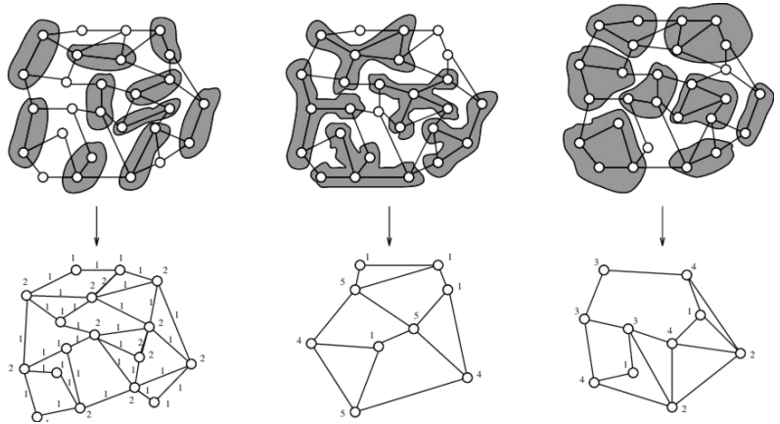

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This talk: graph coarsening and GNNs

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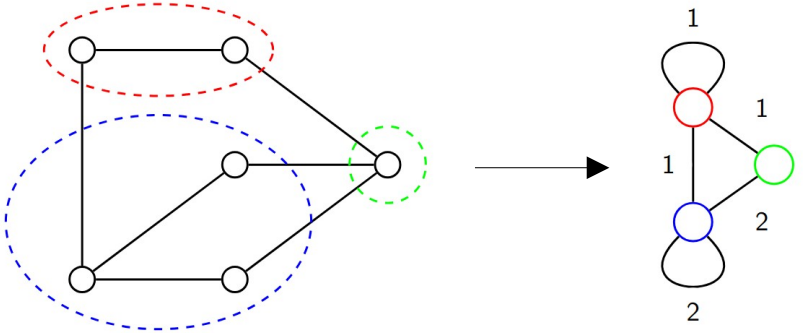
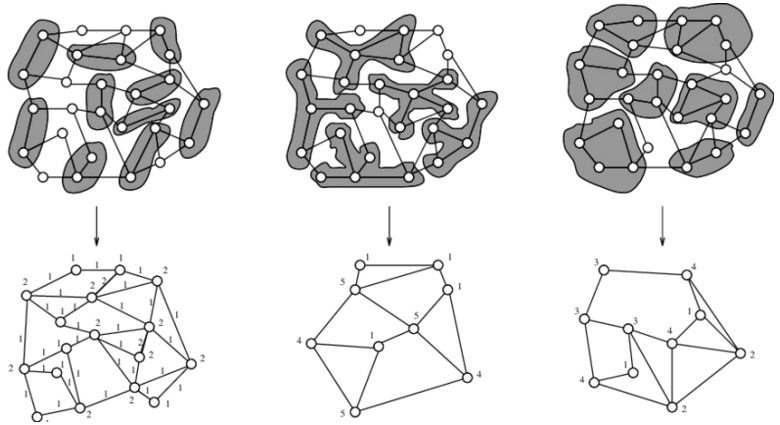


Antonin Joly, Nicolas Keriven, Aline Roumy. **Graph Coarsening with Message-Passing Guarantees** . *NeurIPS 2024*.

Antonin Joly, Nicolas Keriven, Aline Roumy. **Taxonomy of reduction matrices for Graph Coarsening**. *NeurIPS 2025*.



Different ways to coarsen a graph

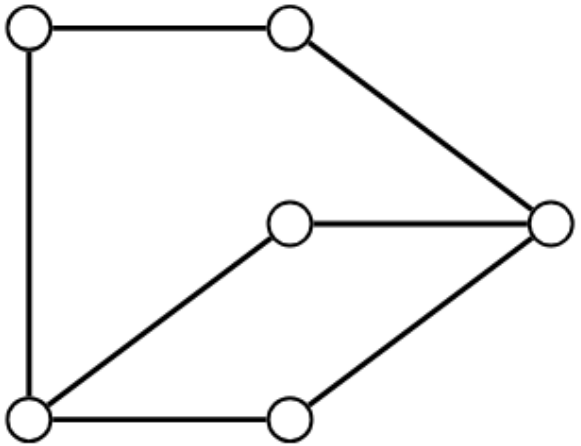
Outline

1. Graph coarsening...
2. ... and Graph Neural Networks
3. Bonus: taxonomy of graph coarsening

Graph

Adjacency matrix

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$



Laplacian

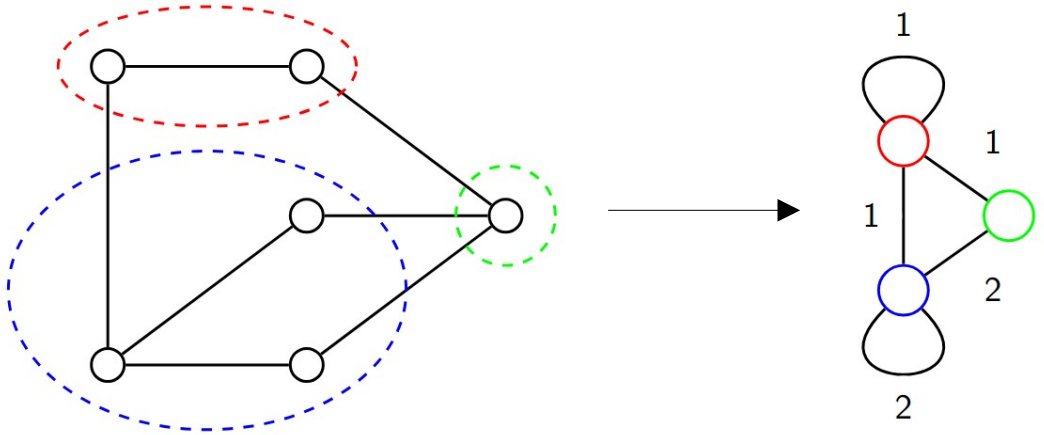
$$L = D - A$$

Diagonal of degrees

Graph coarsening

Graph coarsening:

- group nodes into "**supernodes**"
- Create weighted edges by counting original ones



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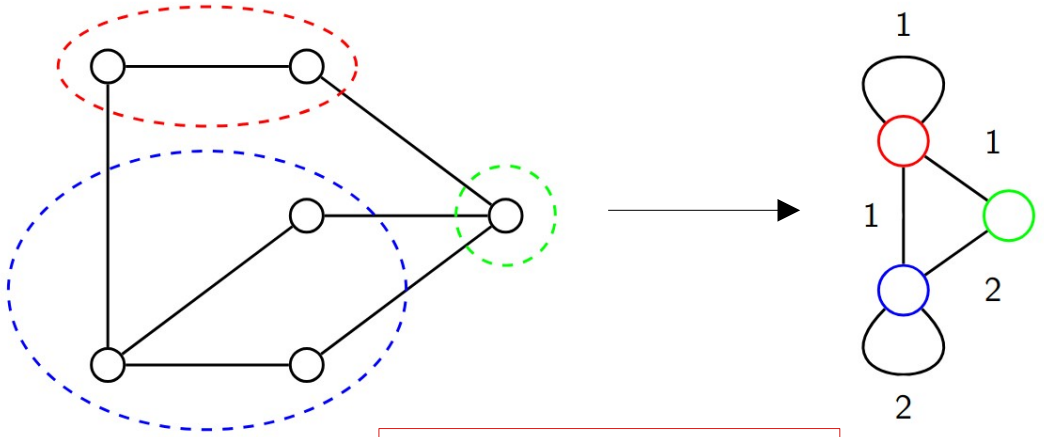

Coarsened Adjacency matrix

$$A_c = Q^\top A Q$$

$$Q = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Membership matrix

Graph coarsening

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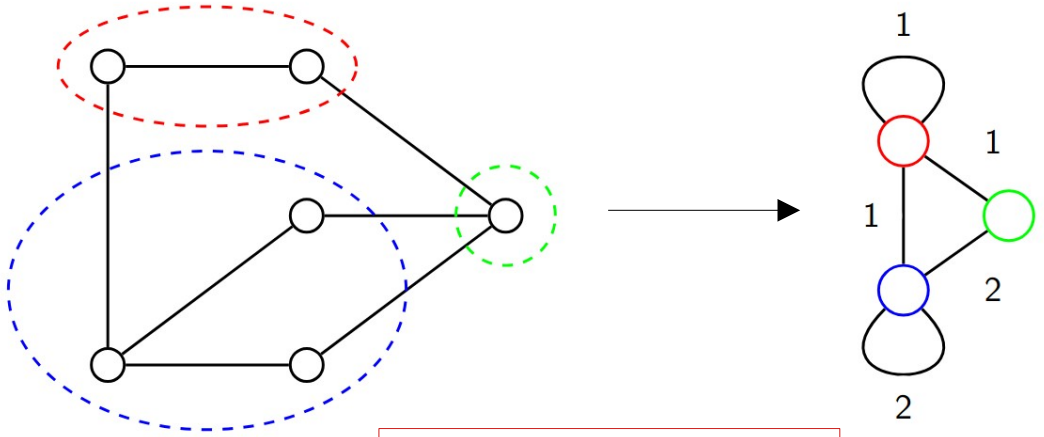


Coarsened Adjacency matrix

$$A_c = Q^\top A Q$$

Coarsened Laplacian

$$L_c = D_c - A_c = Q^\top L Q$$

$$Q = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

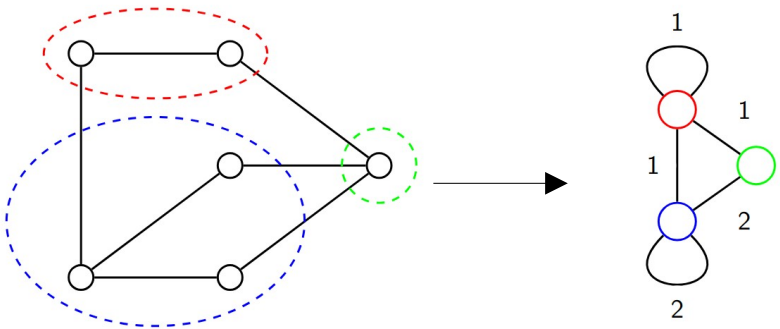
Membership matrix

Graph coarsening consistency

Lemma. (Consistency of Laplacian [1])
Let Q be a well-partitioned matrix. The two following properties are equivalent:

$$Q \text{ is proportional to a binary matrix.}$$
$$\Updownarrow$$
$$\forall A, \quad L(A_c) = Q^\top L Q$$

[1] Andreas Loukas, *Graph Reduction with Spectral and Cut Guarantees*, JMLR 2019.

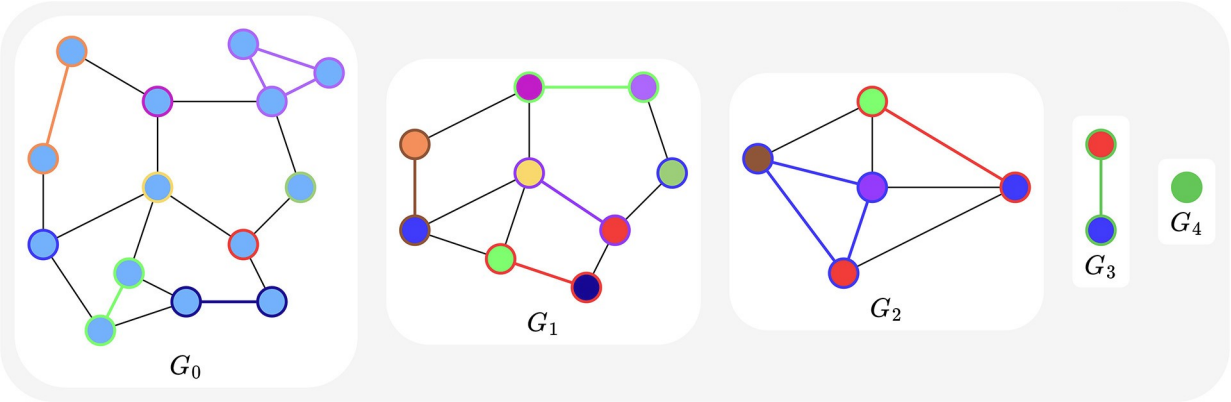


$$Q = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Membership matrix

How to coarsen a graph?

- Many different methods
- Often ***iteratively***
  - Select "contracting set"
    - edges, neighborhood...
  - Merge them
  - Repeat



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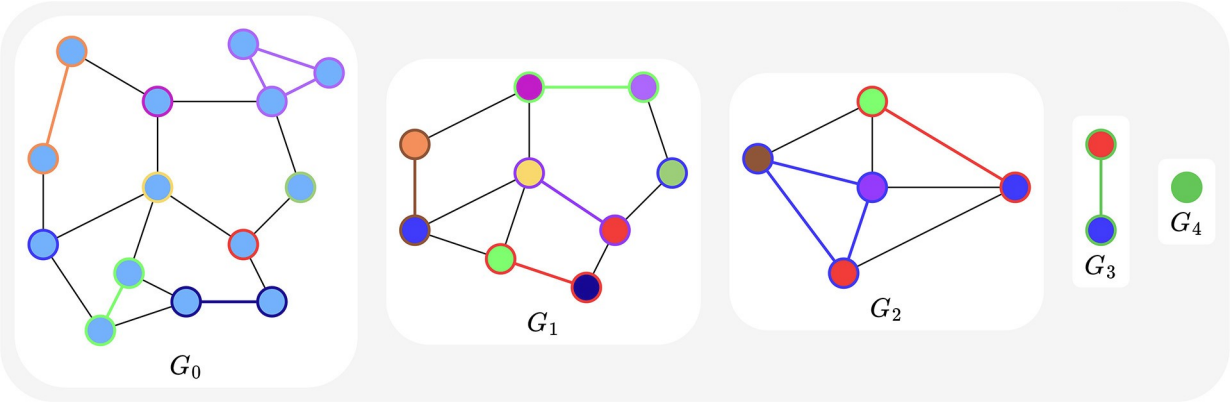

- Generally done to (approximately) optimize some ***cost,*** in a **greedy** manner

Restricted Spectral Approximation

Intuitively, possible to preserve the **low-frequencies** of the graph

- Slow varying ***signals*** $x \in \mathbb{R}^n$ on the big graph can be well-approximated on the small graph

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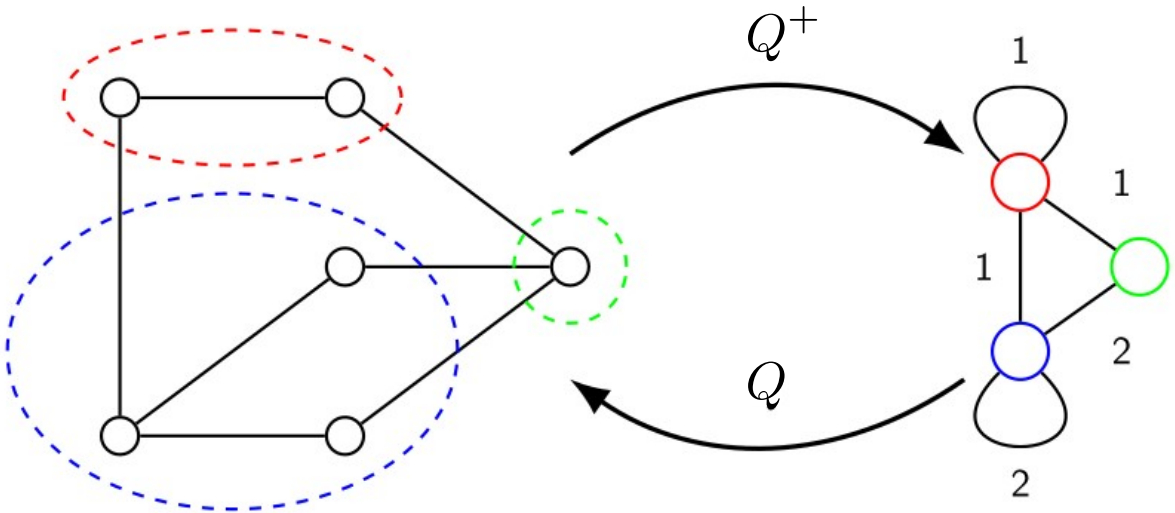

Reduction

$$x_c = Q^+ x$$

Average within super-nodes

Lifting

$$\tilde{x} = Q x_c$$

Expand constant signal within super-nodes

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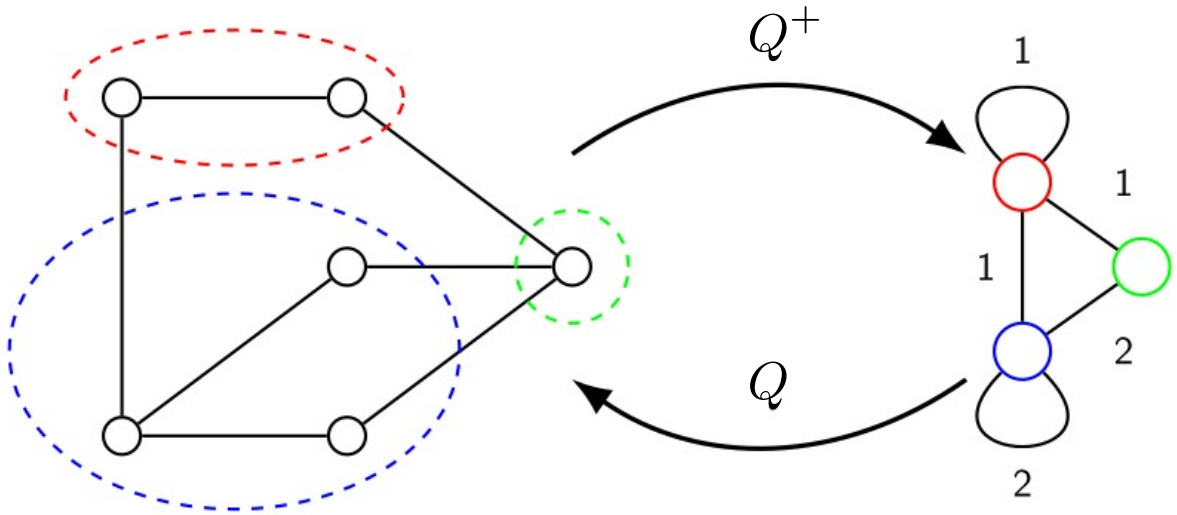

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Does ***reduction-lifting*** degrades too much the signal?

Restricted Spectral Approximation

Speed of variation (aka Dirichlet energy): $$x^\top L x = \sum_{i \sim j} (x_i - x_j)^2 = \|x\|_L^2$$

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RSA: Bound difference between *signal* and **projected-reconstructed version** $\begin{cases} x_c &= Q^+ x \\ \tilde{x} &= Q x_c \end{cases}$

Restricted Spectral Approximation

Speed of variation (aka Dirichlet energy): $x^\top Lx = \sum_{i\sim j}(x_i - x_j)^2 = \|x\|_L^2$

RSA: Bound difference between *signal* and **projected-reconstructed version** $\begin{cases} x_c &= Q^+ x \\ \tilde{x} &= Q x_c \end{cases}$

$$\epsilon_Q = \max_{x\in\mathcal{R}, \|x\|_L=1} \|x - \tilde{x}\|_L$$

some *target* subspace

Consistency: $\|\tilde{x}\|_L = \|x_c\|_{L_c}$

Coarsening algorithm

Goal: $\min_{Q} \epsilon_Q$

Coarsening algorithm

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- NP-hard in general

Coarsening algorithm

Goal: $\min_{Q} \epsilon_Q$

- NP-hard in general
- Approximative algo, often **greedy**
  - Might still be quite costly!

Loukas. *Graph reduction with spectral and cut guarantees* (2019)

Algorithm 2 Single-level coarsening by local variation

input: Combinatorial Laplacian $L_{\ell-1}$, threshold σ', and target size n.
Form the family of candidate sets $\mathcal{F}_\ell = \{\mathcal{C}_1, \mathcal{C}_2, \mathcal{C}_3, \ldots\}$ (algorithm-specific step).
$N_\ell \leftarrow N_{\ell-1}$, marked $\leftarrow \varnothing$, $\sigma_\ell^2 \leftarrow 0$.
Sort $\mathcal{F}_\ell$ in terms of increasing $\text{cost}_\ell(\mathcal{C})$.
while $|\mathcal{F}_\ell| > 0$ and $N_\ell > n$ and $\sigma_\ell \leq \sigma'$ **do**
    Pop the candidate set $\mathcal{C}$ of minimal cost s from $\mathcal{F}_\ell$.
    if all vertices of $\mathcal{C}$ are not marked and $\sigma' \geq \sqrt{\sigma_\ell^2 + (|\mathcal{C}| - 1)s}$ **then**
        marked $\leftarrow$ marked $\cup\, \mathcal{C}$, $\mathcal{P}_\ell \leftarrow \mathcal{P}_\ell \cup \mathcal{C}$, $N_\ell \leftarrow N_\ell - |\mathcal{C}| + 1$, $\sigma_\ell^2 \leftarrow \sigma_\ell^2 + (|\mathcal{C}| - 1)s$
    else
        $\mathcal{C}' \leftarrow \mathcal{C} \setminus$ marked
        if $|\mathcal{C}'| > 1$ **then**
            Compute $\text{cost}_\ell(\mathcal{C}')$ and insert $\mathcal{C}'$ into $\mathcal{F}_\ell$ while keeping the latter sorted.
Form the $N_\ell \times N_{\ell-1}$ coarsening matrix P_ℓ based on $\mathcal{P}_\ell$.
return $L_\ell \leftarrow P_\ell^{\mp} L_{\ell-1} P_\ell^{+}$ and σ_ℓ

Proposition 17 *Matrices L_c and L are $(\mathbf{R}, \epsilon)$-similar with $\epsilon \leq \prod_{\ell=1}^{c}(1 + \sigma_\ell) - 1$.*

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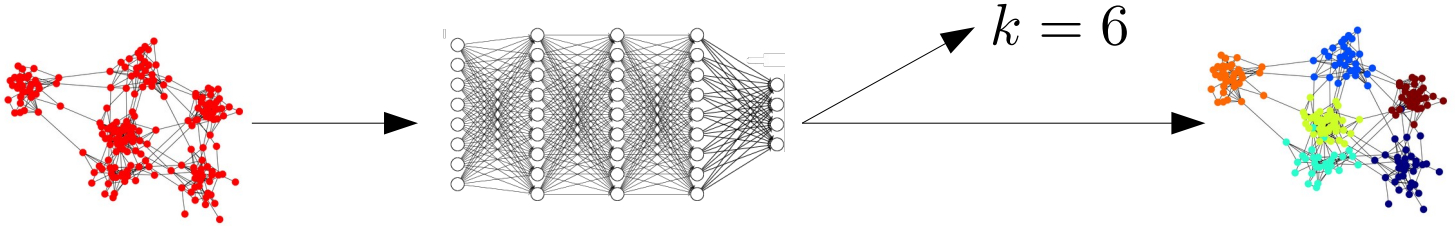
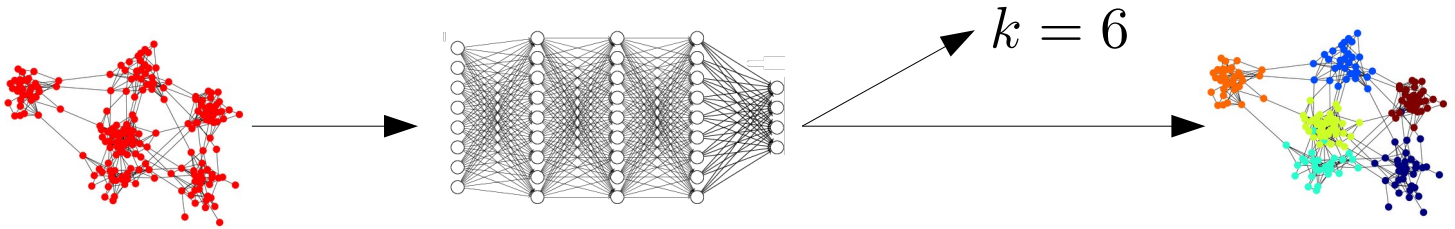
3. Bonus: taxonomy of graph coarsening

ML on graphs: Graph Neural Networks



Graph Neural Networks (GNN) are "deep architectures" to do ML on graphs.

ML on graphs: Graph Neural Networks



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- Updates ***node representations*** at each layer, starting with input **node features**
  - No node features? Handcrafted stuff, but not ideal...

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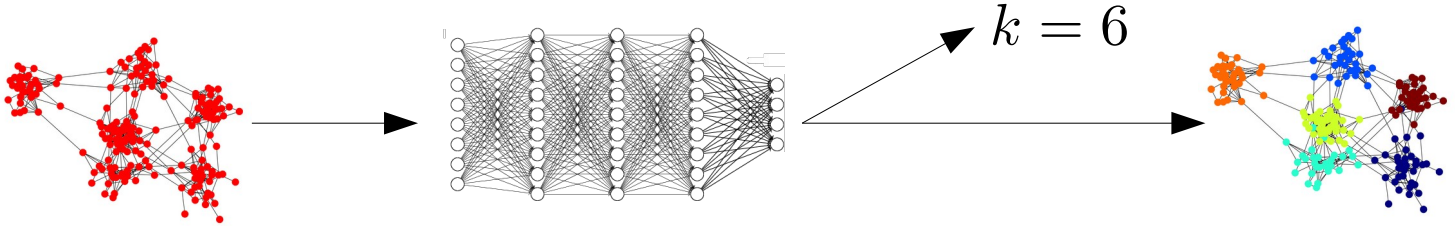

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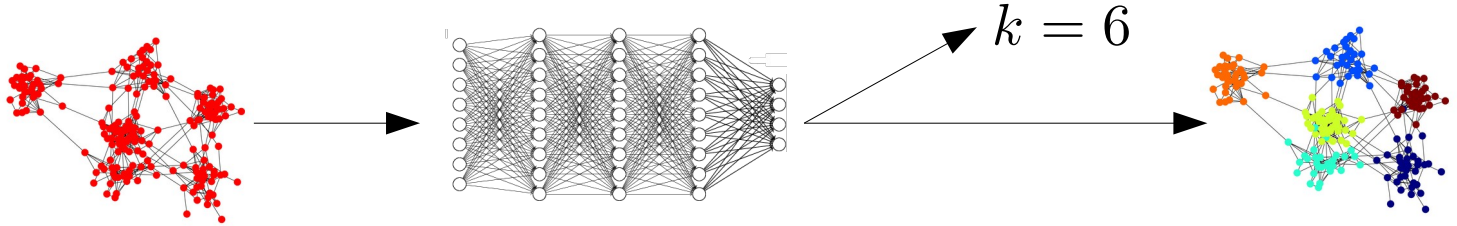

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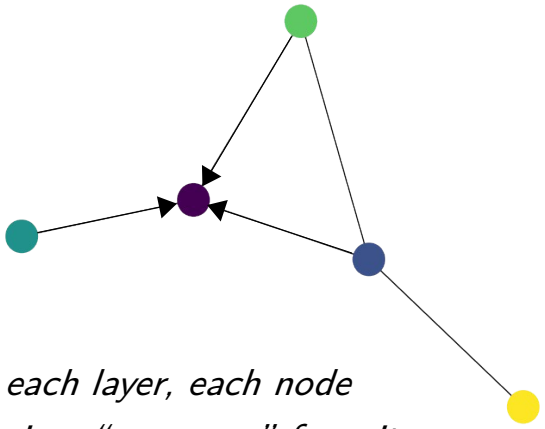
- Updates ***node representations*** at each layer, starting with input **node features**
  - No node features? Handcrafted stuff, but not ideal...
- Alternates linear operations/non-linear activation functions
- Extremely ***flexible***: can perform node/graph/link prediction with minimal adaptation
- State-of-the-art, but still quite many problems

The message-passing paradigm

Modern GNNs are often built around a message-passing interpretation.



At each layer, each node receives "messages" from its neighbors.

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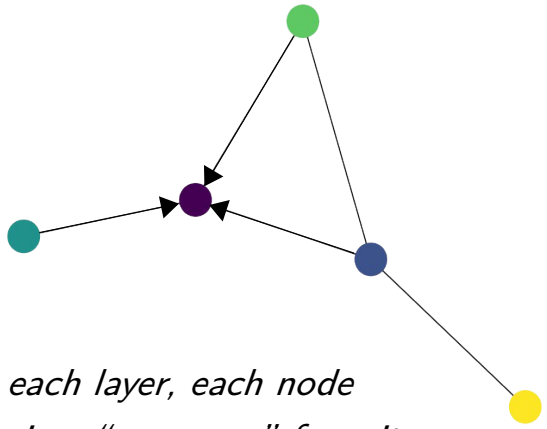

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- $x_i^{(0)}, 1 \leq i \leq n$ *Initial node features*
- $x_i^{(\ell)} = \text{AGGREGATE}\left(x_i^{(\ell-1)}, \{x_j^{(\ell-1)}, a_{ij}\}\right)$
- $\text{output} = \begin{cases} \{x_i^{(L)}\} & \text{(node prediction)} \\ \text{POOL}(\{x_i^{(L)}\}_i) & \text{(graph prediction)} \end{cases}$

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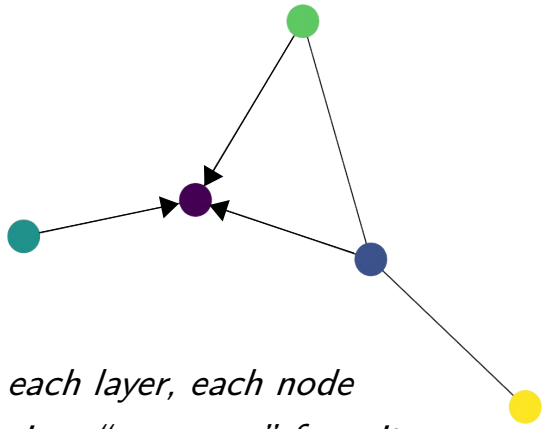

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- Messages are treated as a **set**: no node ordering!
- Resulting GNNs are **permutation equivariant** (node) or **invariant** (graph), and can be applied to ***any graph*** once trained

Propagation matrix

Message-passing often materialized through a ***propagation matrix*** $S \in \mathbb{R}^{n \times n}$, such that

$$X^{(\ell)} = \sigma\left(SX^{(\ell-1)}W^{(\ell)} + 1_n b_\ell^\top\right)$$

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$$S = A \rightarrow x_i^{(\ell)} = \sigma\left({W^{(\ell)}}^\top \sum_{j \sim i} x_j^{(\ell-1)} + b_\ell\right) \qquad \textit{(sum aggregation)}$$

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$$S = D^{-1}A \rightarrow x_i^{(\ell)} = \sigma\left(W^{(\ell)^\top} \frac{1}{d_i} \sum_{j \sim i} x_j^{(\ell-1)} + b_\ell\right) \quad \textit{(mean aggregation)}$$

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$$S = D^{-1/2}AD^{-1/2} \to x_i^{(\ell)} = \sigma\left(W^{(\ell)\top} \frac{1}{\sqrt{d_i}} \sum_{j \sim i} \frac{x_j^{(\ell-1)}}{\sqrt{d_j}} + b_\ell\right)$$

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- **Within** the GNN itself -> may be differentiable
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- GNN can also be *trained* to coarsen graphs
  - Cai et al. *Graph coarsening with neural networks.* 2021

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- Assuming a good RSA? (good quality coarsening)
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Boils down to: is propagating with S approximately the same as propagating with S_c ?

Choice of coarsened propagation

Natural/previous choice: if $S = f(A)$, take $S_c = f(A_c)$

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Does not work! Example: $S = A, S_c = A_c = Q^\top A Q$

Coarsening, reconstruction

$$QX_c = \underbrace{QQ^+}_{RSA} X \quad \text{is approximately } X$$

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Coarsening, ***propagation,*** *reconstruction*

$$QA_cX_c = \underbrace{QQ^\top}_{???} A \underbrace{QQ^+}_{RSA} X \quad \text{is } \textbf{\textit{not}} \text{ approximately } AX$$

Immediate fix!

Simple fix! $\boxed{S_c = Q^+ S Q}$

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Simple fix! $\boxed{S_c = Q^+ S Q}$ Then $QS_cX_c = \underbrace{QQ^+}_{RSA} S \underbrace{QQ^+}_{RSA} X \approx SX$

Can be transferred to guarantees on GNN training under appropriate assumptions...

Assumptions

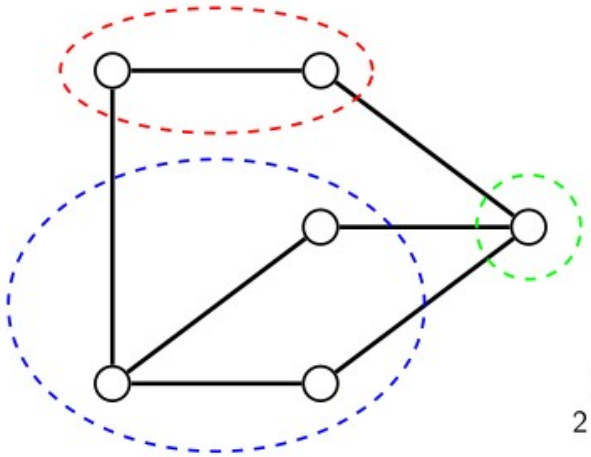
- There is a constant C_J such that $|J(x) - J(x')| \leq C_J \|x - x'\|_L$, with J the loss function
- σ is $\mathcal{R}$-preserving, that is, for all $x \in \mathcal{R}$, we have $\sigma(x) \in \mathcal{R}$, $\|\sigma(x) - \sigma(x')\|_L \leq C_\sigma \|x - x'\|_L$, σ and Q^+ commute: $\sigma(Q^+ y) = Q^+ \sigma(y)$.

For all node features $X \in \mathbb{R}^{N \times d}$ such that $X_{:,i} \in \mathcal{R}$, denoting by $\theta^\star = \arg\min_{\theta \in \Theta} R(\theta)$ and $\theta_c = \arg\min_{\theta \in \Theta} R_c(\theta)$, we have

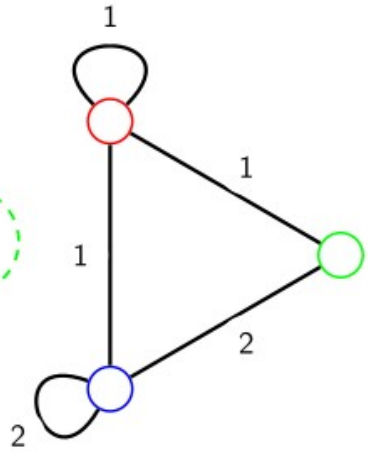
$$\boxed{R(\theta_c) - R(\theta^\star) \leq C \epsilon_{L,Q,\mathcal{R}} \|X\|_{:,L}}$$

Properties

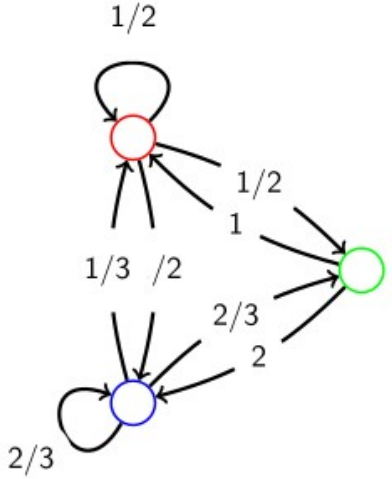
$$S_c = Q^+ S Q$$



$S = A$



$S_c = A_c$

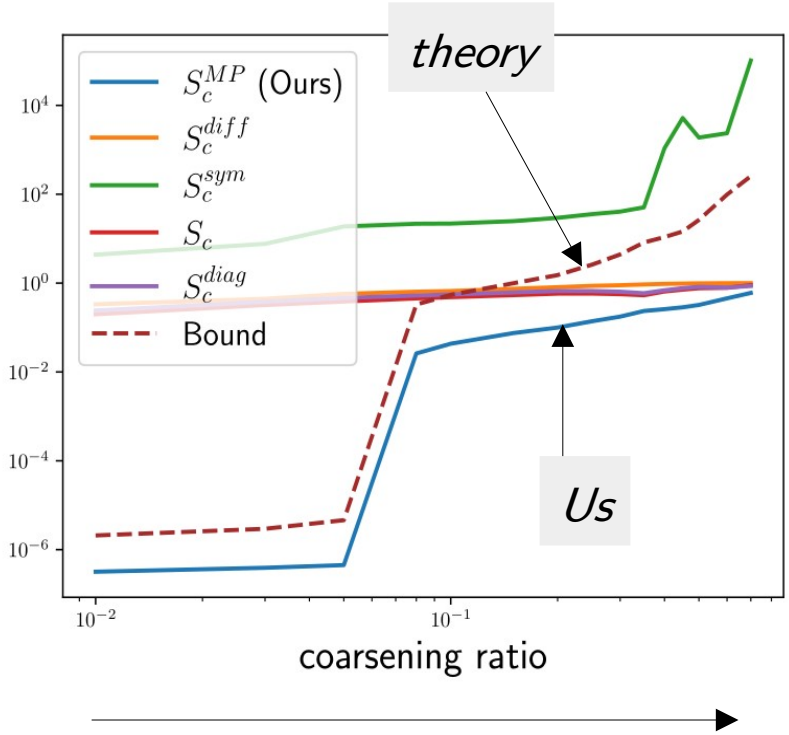


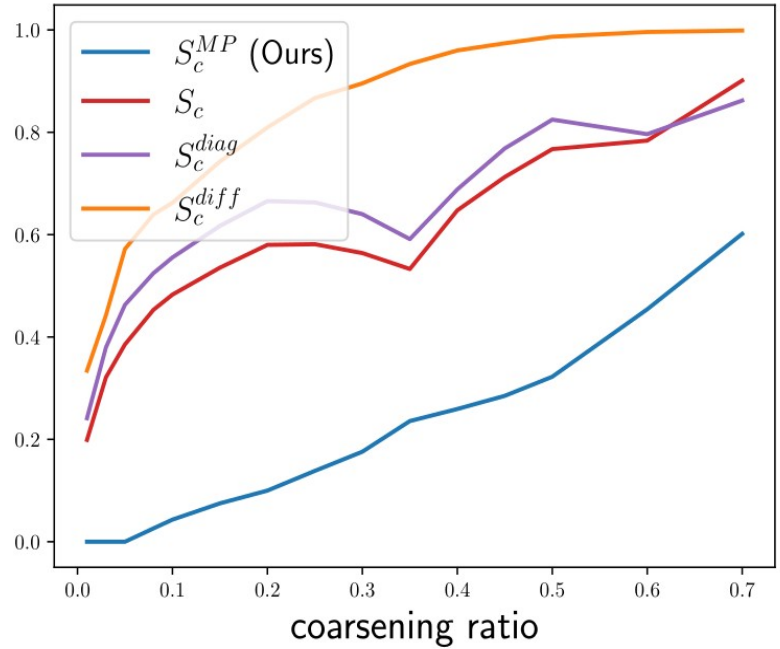
$S_c = Q^+ A Q$

- ***Not symmetric*** in general!
- Twice the memory footprint (mild)
- Can be applied to any propagation matrix!

Numerical results

Approx error





Smaller graph

Numerical Results

Dataset	# Nodes	# Edges	# Features	#classes
Reddit	232,965	114,615,892	602	41
Reddit90	23,298	8,642,864	602	41
Reddit99	2,331	10,838	602	41
Cora PCC	2,485	10,138	1,433	7
Cora70	746	3,716	1,433	7
Citeseer PCC	2,120	7,358	3,703	6
Citeseer70	636	2,122	3,703	6

SGC	Cora		Citeseer		Reddit	
r	0.5	0.7	0.5	0.7	0.9	0.99
S_c^{sym}	16.1 ± 3.8	16.4 ± 4.7	18.6 ± 4.6	19.8 ± 5.0	37.1 ± 6.6	3.7 ± 5.5
S_c^{diff}	21.8 ± 2.2	13.6 ± 2.8	30.5 ± 0.2	23.1 ± 0.0	18.3 ± 0.0	14.9 ± 0.0
S_c	78.7 ± 0.0	74.6 ± 0.1	72.8 ± 0.1	72.5 ± 0.1	87.5 ± 0.1	37.3 ± 0.0
S_c^{diag}	78.7 ± 0.1	77.3 ± 0.0	73.4 ± 0.1	73.1 ± 0.4	87.6 ± 0.1	37.3 ± 0.0
S_c^{MP} **(ours)**	**80.3** ± 0.1	**78.5** ± 0.0	**74.6** ± 0.1	**74.2** ± 0.1	**90.2** ± 0.0	**64.1** ± 0.0
Full Graph	81.6 ± 0.1		73.6 ± 0.0		94.9	

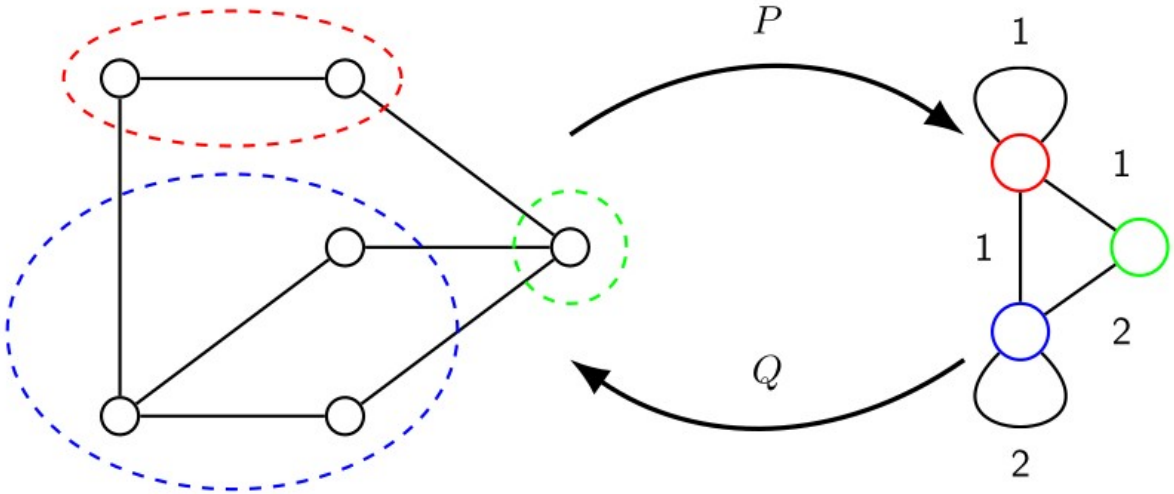
GCNconv	Cora		Citeseer		Reddit	
r	0.5	0.7	0.5	0.7	0.9	0.99
S_c^{sym}	78.1 ± 1.3	30.8 ± 2.5	62.5 ± 11	52.7 ± 3.6	48.1 ± 8.9	34.8 ± 4.0
S_c^{diff}	74.5 ± 0.9	62.6 ± 7.1	71.2 ± 1.7	37.6 ± 0.9	71.3 ± 1.0	18.7 ± 1.7
S_c	79.9 ± 0.9	78.1 ± 1.0	70.7 ± 1.0	67.1 ± 3.1	88.0 ± 0.1	54.2 ± 2.4
S_c^{diag}	**80.4** ± 0.8	**78.6** ± 1.3	70.2 ± 0.8	69.3 ± 1.9	**88.1** ± 0.2	55.5 ± 1.8
S_c^{MP} **(ours)**	79.8 ± 1.5	78.2 ± 0.9	**72.0** ± 0.8	**70.0** ± 1.0	84.4 ± 0.3	**60.3** ± 0.9
Full Graph	81.6 ± 0.6		73.1 ± 1.5		OOM	

-> difficult to treat ***very large graphs***, as the RSA-coarsening itself is costly... (future work)

Outline

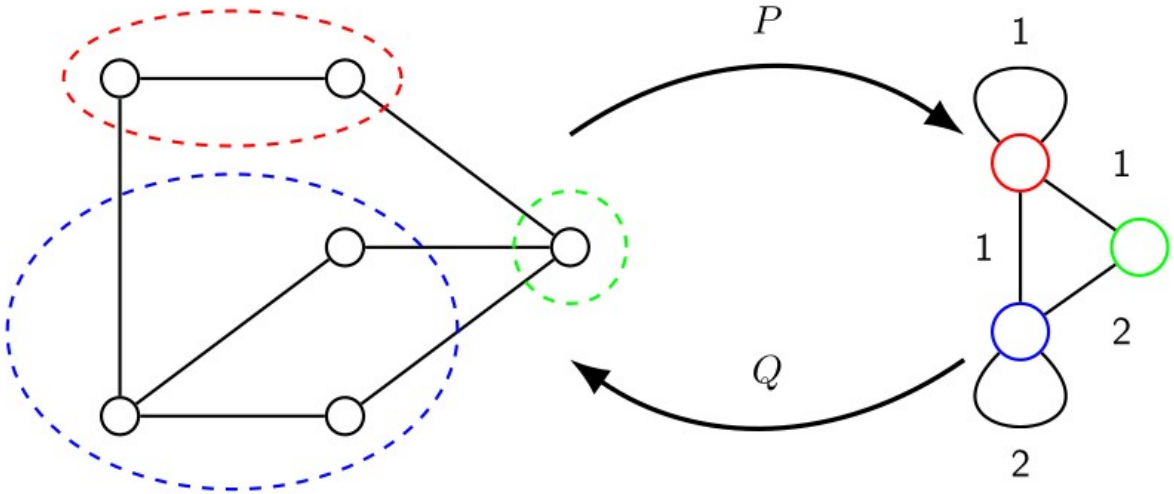
1. Graph coarsening...
2. ... with Graph Neural Networks
3. Bonus: taxonomy of graph coarsening

Reduction vs lifting



- Until now, $P = Q^+$

Reduction vs lifting



- Until now, $P = Q^+$
- But only Q is important for consistency!
- **Can we change P?**

Lemma. (Consistency of Laplacian [1])
Let Q be a well-partitioned matrix. The two following properties are equivalent:

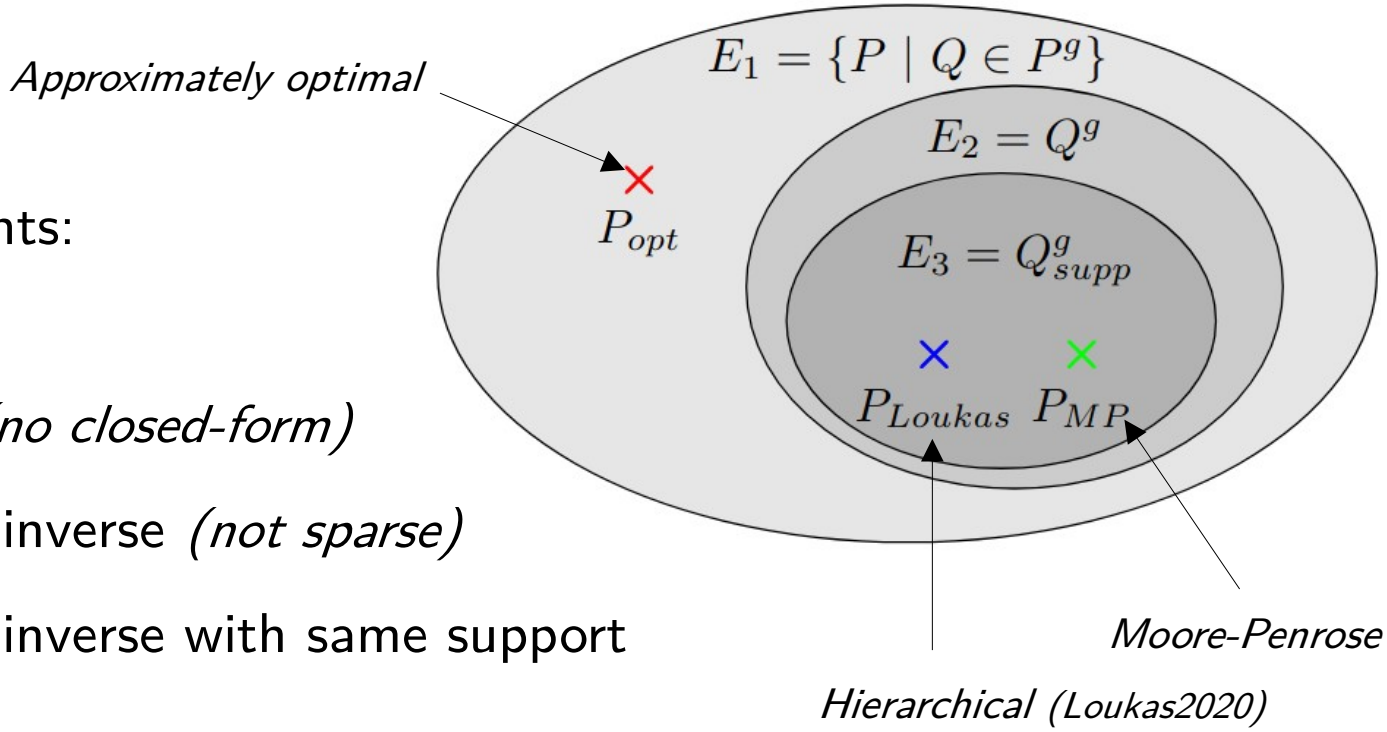
$$Q \text{ is proportional to a binary matrix.}$$
$$\Updownarrow$$
$$\forall A, \quad L(A_c) = Q^\top L Q$$

[1] Andreas Loukas, *Graph Reduction with Spectral and Cut Guarantees*, JMLR 2019.

Several choices for P

Increasing level of constraints:

- E1: Generalized inverse *(no closed-form)*
- E2: Generalized reflexive inverse *(not sparse)*
- E3: Generalized reflexive inverse with same support



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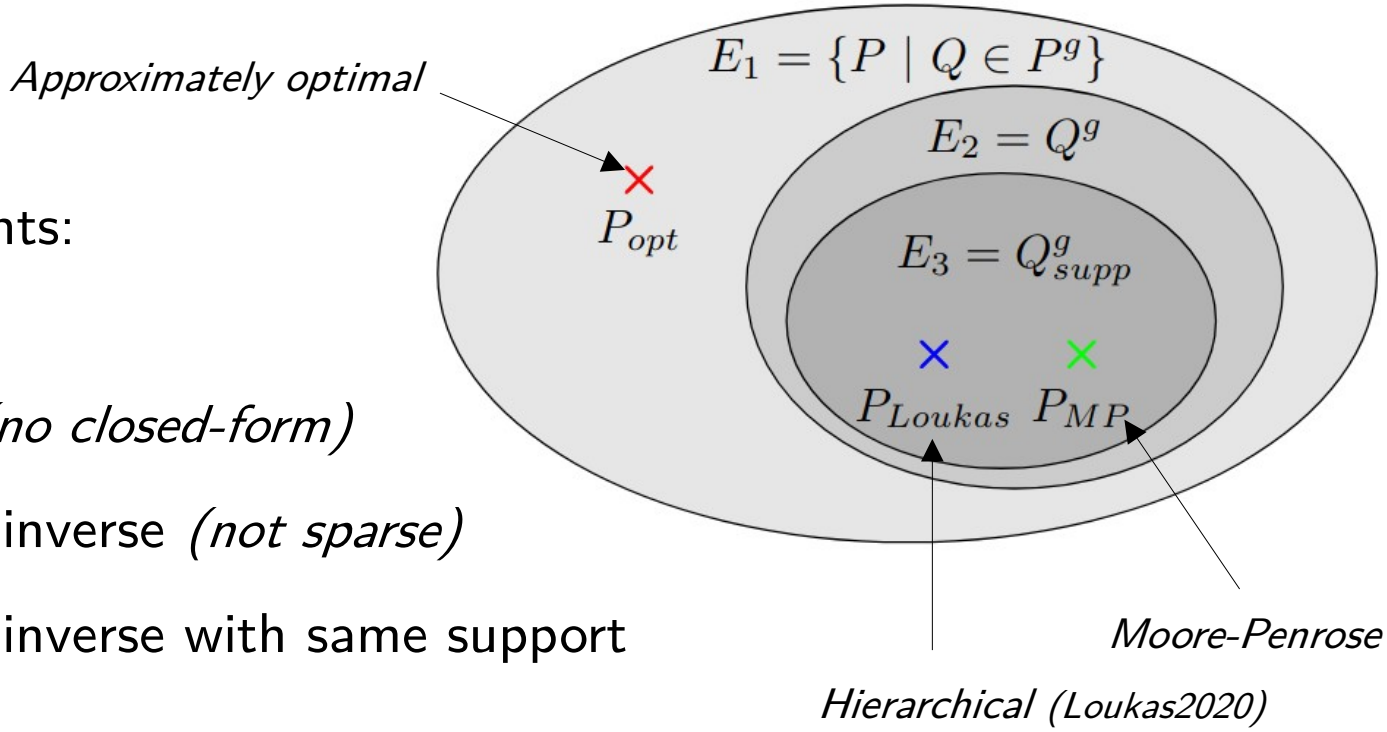
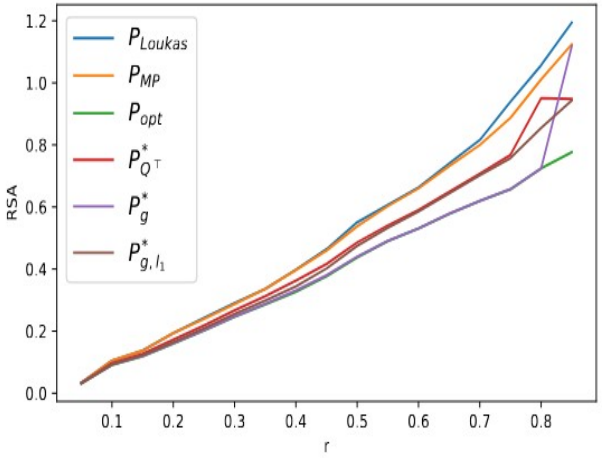


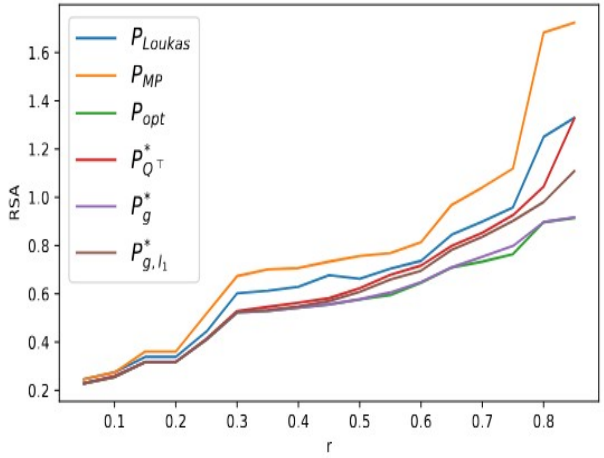
-> closed-form (E2 and 3) can be used to ***optimize*** the RSA!

Several choices for P

-> can be used to ***further optimize*** the RSA!



(a) Cora graph, combinatorial Laplacian $\mathcal{L}$



(b) Cora graph, self-loop normalized Laplacian L

SGC	Cora			Citeseer		
r	0.3	0.5	0.7	0.3	0.5	0.7
P_{Loukas}	80.5 ± 0.0	79.7 ± 0.0	76.8 ± 0.0	72.6 ± 0.3	71.7 ± 0.1	**69.7** ± 0.7
P_{MP}	80.5 ± 0.0	**80.1** ± 0.0	77.7 ± 0.0	72.8 ± 0.5	72.7 ± 0.0	69.5 ± 0.3
P_{opt}	77.1 ± 0.6	75.9 ± 0.1	73.8 ± 0.3	70.9 ± 0.2	70.2 ± 0.1	67.3 ± 0.4
$P^*_{Q^\top}$	80.3 ± 0.0	80.0 ± 0.1	77.2 ± 0.0	72.7 ± 0.3	72.6 ± 0.5	67.6 ± 0.2
P^*_g	**80.7** ± 0.0	80.0 ± 0.0	77.6 ± 0.0	72.6 ± 0.2	**72.7** ± 0.0	68.6 ± 0.4
P^*_{g,l_1}	80.4 ± 0.0	79.2 ± 0.0	**78.3** ± 0.0	**73.0** ± 0.0	71.2 ± 0.1	69.2 ± 0.4
Full Graph		81.0 ± 0.1			71.6 ± 0.1	

GCN	Cora			Citeseer		
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P_{MP}	80.4 ± 1.0	80.7 ± 0.9	78.6 ± 0.9	70.8 ± 1.9	72.1 ± 1.0	**71.0** ± 1.0
P_{opt}	73.7 ± 1.5	63.3 ± 1.4	55.11 ± 2.4	64.6 ± 0.7	50.4 ± 1.6	42.6 ± 4.0
$P^*_{Q^\top}$	80.5 ± 0.9	80.9 ± 0.6	78.0 ± 0.9	**71.1** ± 1.5	**72.3** ± 0.7	70.0 ± 0.9
P^*_g	**80.6** ± 1.1	**81.3** ± 0.6	**78.7** ± 0.9	**71.1** ± 1.7	72.1 ± 1.2	69.6 ± 1.0
P^*_{g,l_1}	80.4 ± 0.9	80.0 ± 0.9	78.2 ± 0.7	70.2 ± 1.8	66.8 ± 1.1	66.7 ± 1.2
Full Graph		81.3 ± 0.8			70.9 ± 1.4	

Can be used within GNNs

Outline

Conclusion

Conclusion

- ***Graph reduction*** is unavoidable in Graph Machine Learning, but still in its infancy
- Both **coarsening** and **sampling** have pros and cons
- Graph coarsening is *difficult/costly*, but bears many promising directions
  - pooling CNN-like? **Heterogeneous graphs?**

Antonin Joly, Nicolas Keriven, Aline Roumy. **Graph Coarsening with Message-Passing Guarantees** . *NeurIPS 2024*.

Antonin Joly, Nicolas Keriven, Aline Roumy. **Taxonomy of reduction matrices for Graph Coarsening**. *NeurIPS 2025*.

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