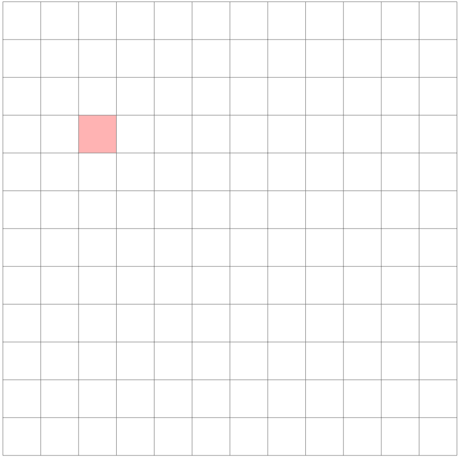
Pooling in Graph Neural Networks

Graph Deep Learning 2021 - Lecture 4

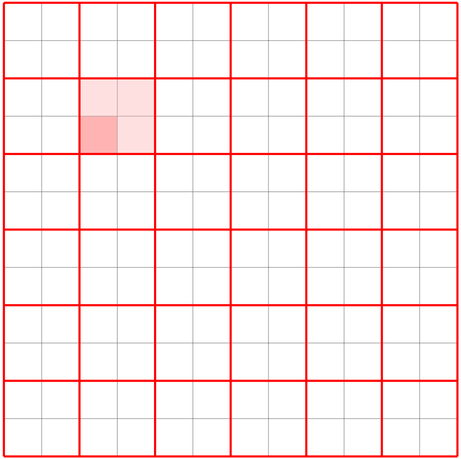
Daniele Grattarola

March 15, 2021

Pooling in CNNs



Pooling in CNNs



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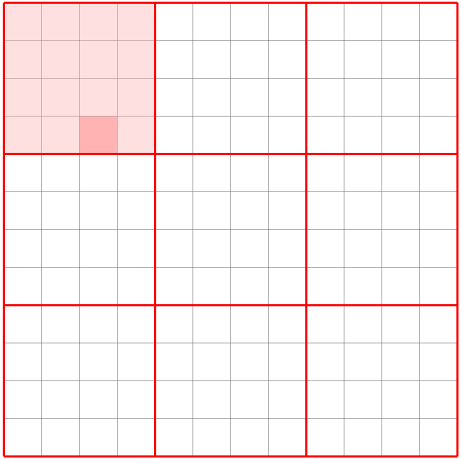

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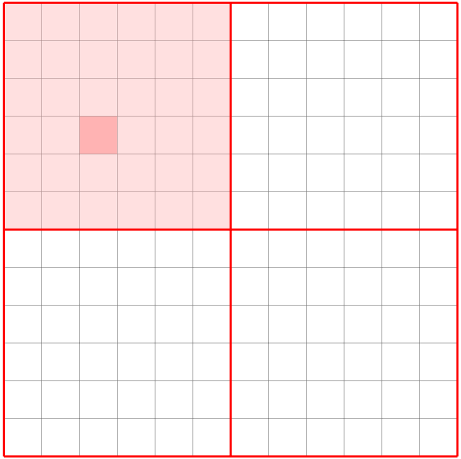

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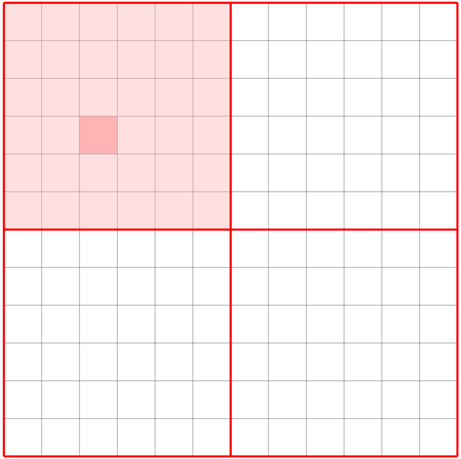

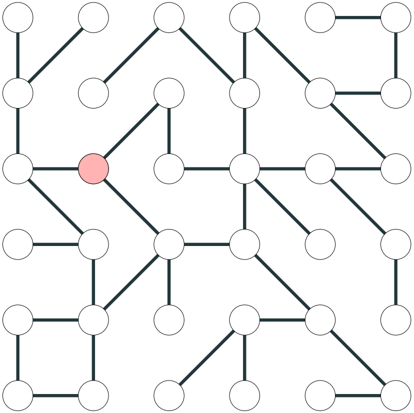

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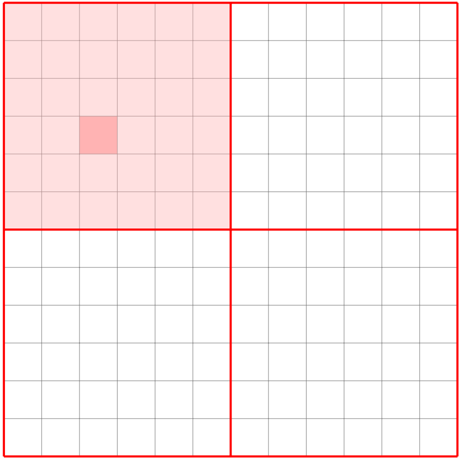

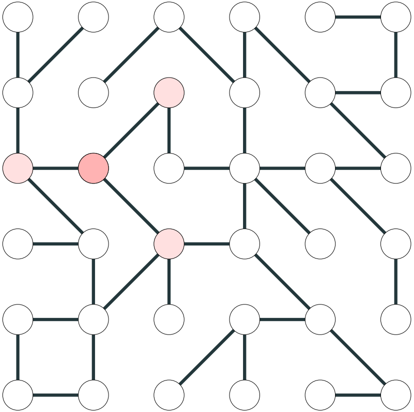

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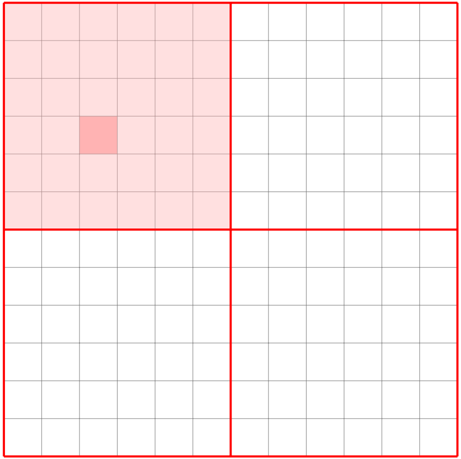

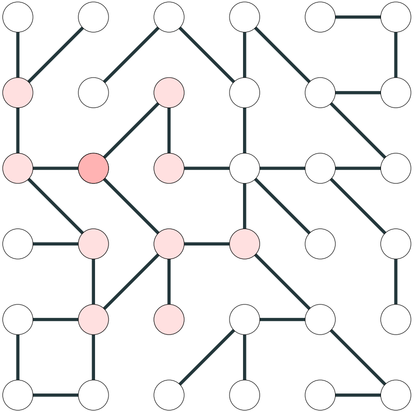

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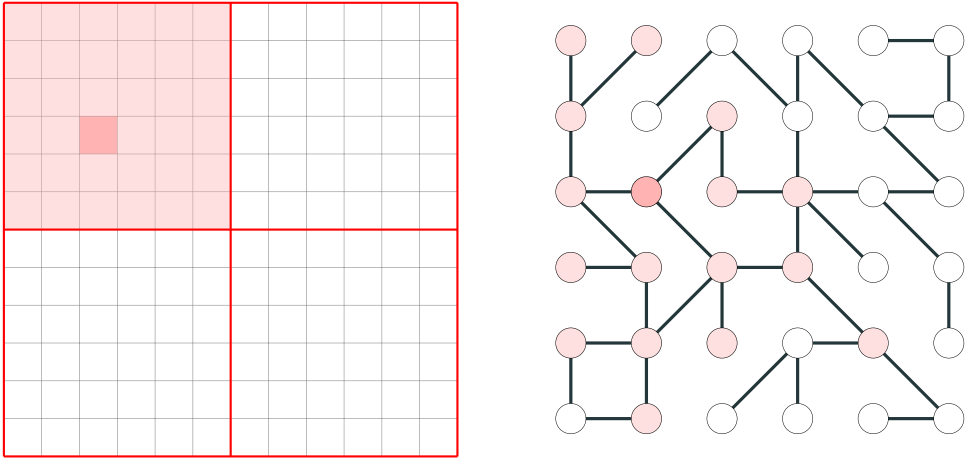


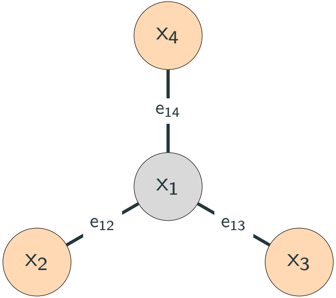
Roadmap

Things we are going to cover:

- A “message passing” for pooling
- Methods
- Global pooling
- Open questions

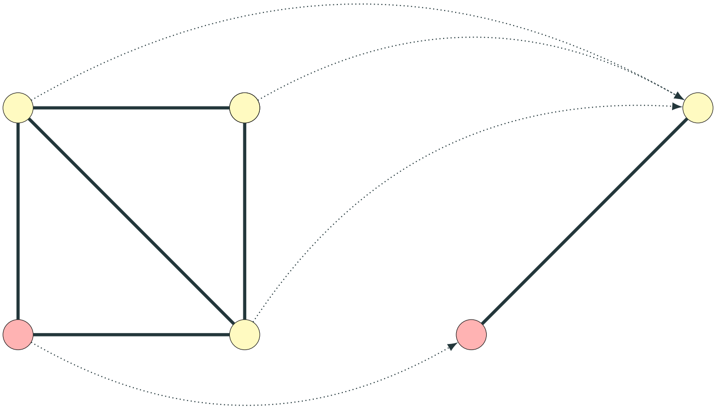
Notation recap

- Graph: nodes connected by edges;
- A, $N \times N$ adjacency matrix;
- $\mathrm{D} = \mathrm{diag}([d_1, \dots, d_N])$, diagonal degree matrix;
- $\mathrm{X} = [\mathrm{x}_1, \dots, \mathrm{x}_N]$, $\mathrm{x}_i \in \mathbb{R}^F$, node attributes or "graph signal";
- $\mathrm{e}_{ij} \in \mathbb{R}^S$, edge attribute for edge $i \to j$;



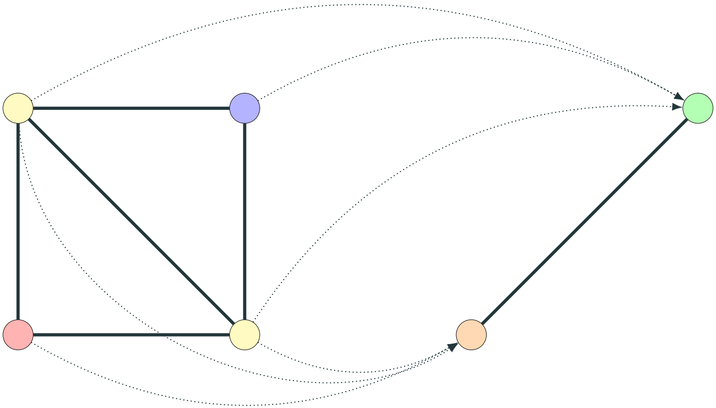
Graph coarsening by example

Strategy 1: aggregate same attributes (Candy Crush pooling).



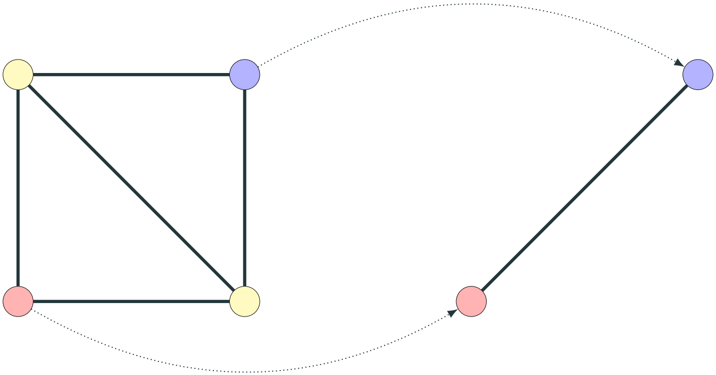
Graph coarsening by example

Strategy 2: aggregate cliques.



Graph coarsening by example

Strategy 3: keep only some types/colors.



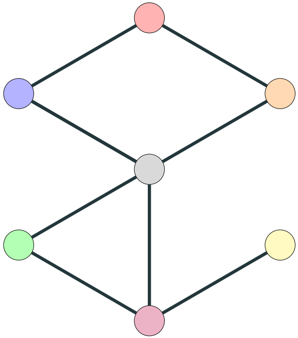
Three main questions [1]

1. How to identify **groups of related nodes**?
2. How to get **new node attributes** from the groups?
3. How to **connect** the new nodes?

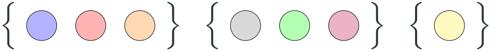
[1] D. Grattarola *et al.*, "Understanding Pooling in Graph Neural Networks," 2021 (In preparation).

Step 1: Select

Selecting nodes



Example 1: partition.



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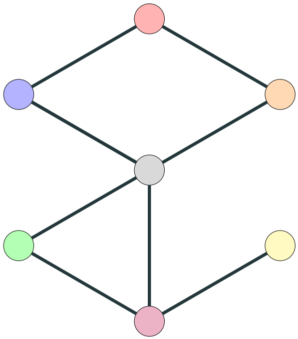

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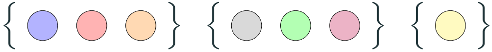
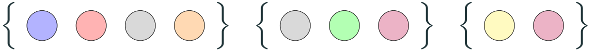


Example 2: cover (possible overlaps).



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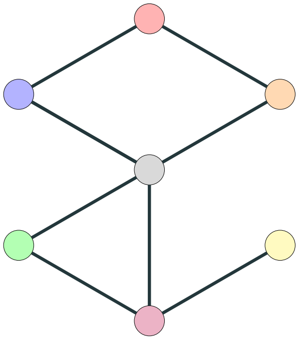

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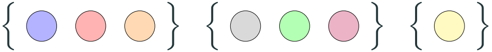

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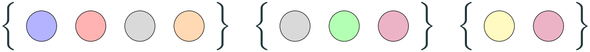
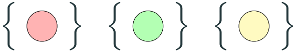


Example 3: sparse.



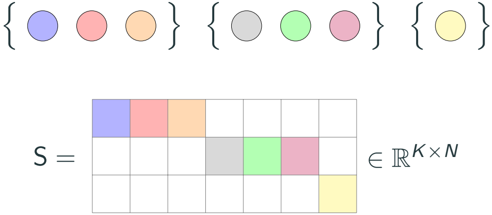
Selecting nodes

The **selection** stage computes K **supernodes**:

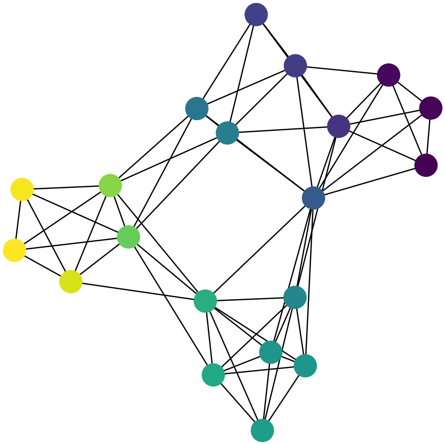
$$\mathrm{Sel} : \mathcal{G} \mapsto \mathcal{S} = \{\mathcal{S}_1, \dots, \mathcal{S}_K\}.$$

Each supernode is a set of nodes associated with a score:

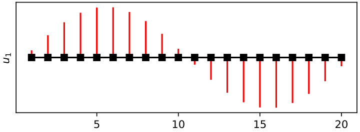
$$\mathcal{S}_k = \{(\mathrm{x}_i, \mathrm{s}_i) \mid \mathrm{s}_i \in \mathbb{R}_{>0}\},$$



Spectral clustering [3]



The low-frequency eigenvectors naturally cluster the nodes.



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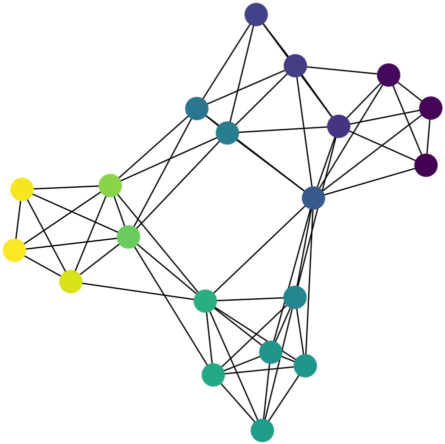

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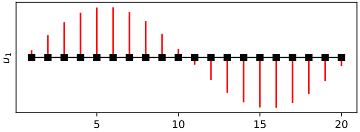

Idea: run k-means clustering (or similar) using the first few eigenvectors.

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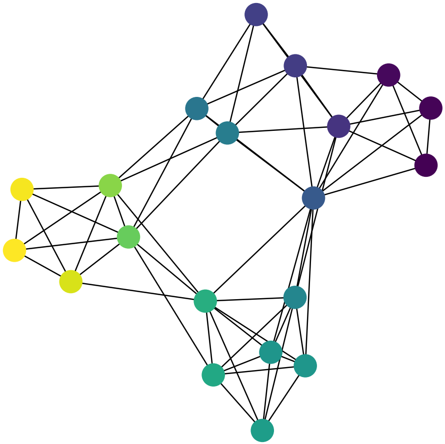

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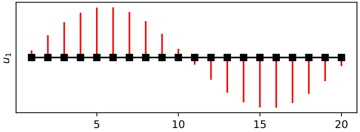

Idea: run k-means clustering (or similar) using the first few eigenvectors.

Equivalent to finding the **minimum normalized k-cut** [2].

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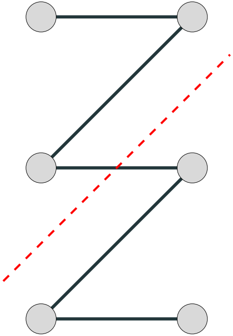
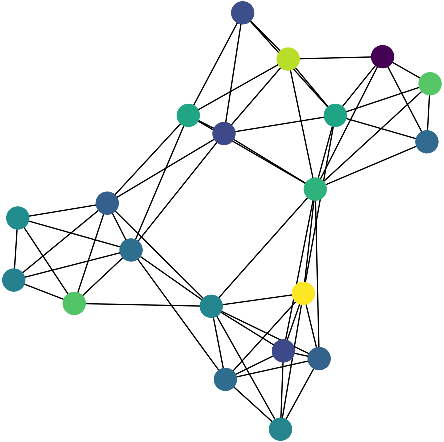
Mincut vs. Maxcut

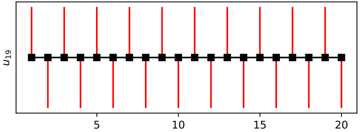


Mincut

Node decimation [5]



Alternative: use the highest-frequency eigenvector to do something similar to a regular subsampling.



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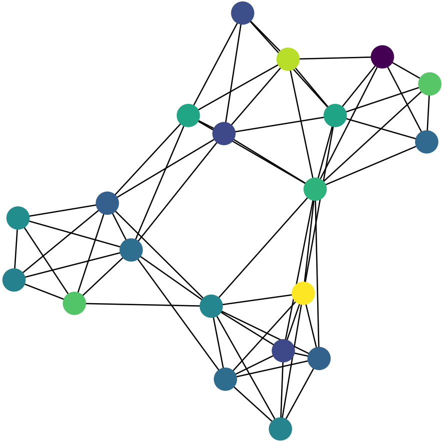

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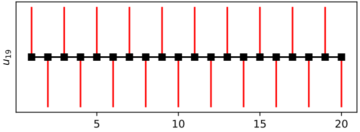

Equivalent to finding the **maximum 2-cut** [4].

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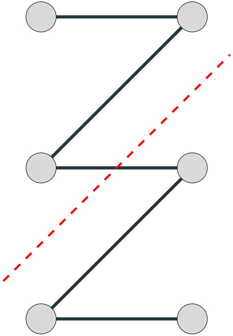
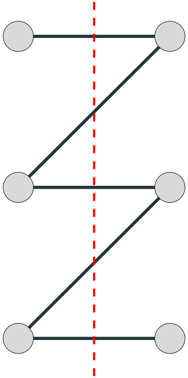
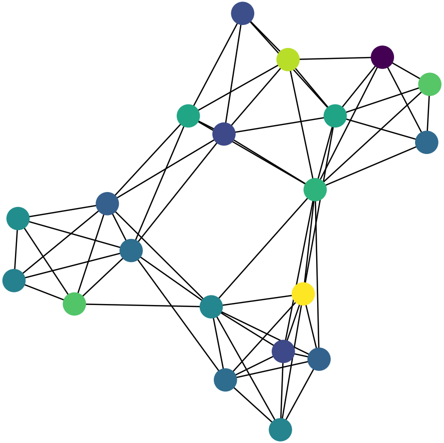


Mincut



Maxcut

Some problems



Problems with spectral methods:

- Computing eigenvectors is **expensive** ($O(N^3)$);
- They do not consider **attributes**.

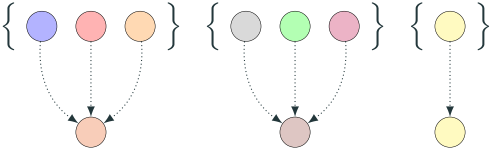
But we get the general idea...

Step 2: Reduce

Reducing supernodes

The **reduction** stage aggregates the supernodes in a **permutation-invariant** way:

$$\text{Red} : \mathcal{G}, \mathcal{S}_k \mapsto \mathrm{x}'_k$$



Typical approach is to take a **weighted sum** (weights given by the scores in the supernodes):

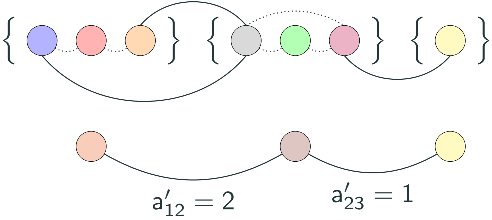
$$\mathrm{X}' = \mathrm{S}\mathrm{X} \quad (\in \mathbb{R}^{K \times F})$$

Step 3: Connect

Connecting supernodes

The **connection** function decides whether two supernodes are connected (and, in case, computes the associated attributes):

$$\text{Con} : \mathcal{G}, \mathcal{S}_k, \mathcal{S}_l \mapsto e'_{kl}$$



Typical approach is again to take a **weighted sum** of edges between two supernodes:

$$A' = SAS^\top \quad (\in \mathbb{R}^{K \times K})$$

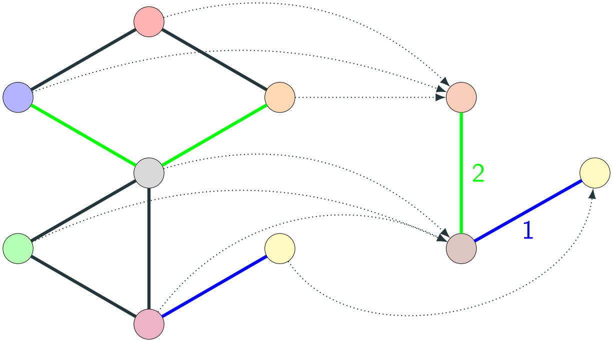
Select, Reduce, Connect [1]

Putting everything together:

$$\underbrace{\mathcal{S} = \{\mathcal{S}_k\}_{k=1:K} = \mathrm{Sel}(\mathcal{G});}_{\text{Selection}}$$

$$\underbrace{\mathcal{X}' = \{\mathrm{Red}(\mathcal{G}, \mathcal{S}_k)\}_{k=1:K};}_{\text{Reduction}}$$

$$\underbrace{\mathcal{E}' = \{\mathrm{Con}(\mathcal{G}, \mathcal{S}_k, \mathcal{S}_l)\}_{k,l=1:K};}_{\text{Connection}}$$



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Methods

Pooling methods

A few ideas:

1. **Graclus** [6]: visit nodes randomly, merge pairs that maximize $\frac{a_{ij}}{w_i} + \frac{a_{ij}}{w_j}$; [1]

   In [7], they reduce supernodes with element-wise max.

[6] I. S. Dhillon *et al.*, "Weighted graph cuts without eigenvectors a multilevel approach," 2007.
[7] M. Defferrard *et al.*, "Convolutional neural networks on graphs with fast localized spectral filtering," 2016.
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[1] w_i is a "weight" assigned to the node, *e.g.*, its degree.

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3. **LaPool** [9]: select "leaders" that have higher local variation $\|LX\|$ w.r.t. all their neighbors. Create clusters by assigning nodes to nearest leader.

---

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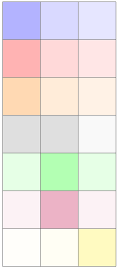
Learning to pool

Key idea: learn to output $S^\top$ by giving node features X as input to a neural network.

- **DiffPool** [10]: GNN for $S^\top$, regularize with "link prediction" loss;

$\phi(X) = S^\top =$  $\in \mathbb{R}^{N \times K}$

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[12] C. Bodnar *et al.*, "Deep Graph Mapper: Seeing Graphs through the Neural Lens," 2020.

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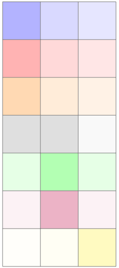
$\phi(\mathsf{X}) = \mathsf{S}^\top =$  $\in \mathbb{R}^{N\times K}$

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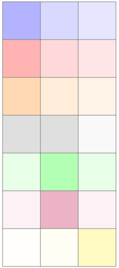
- **MinCutPool** [11]: MLP for $S^\top$, regularize with “minimum cut” loss (same objective as spectral clustering);
- **Deep Graph Mapper** [12]: combine Mapper [13] and GCN [14] to compute clusters.

$\phi(X) = S^\top =$  $\in \mathbb{R}^{N \times K}$

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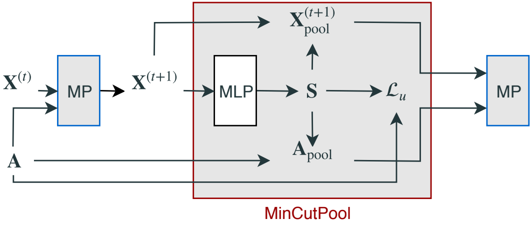
MinCut Pooling [11]

- Select: $S^\top = \mathrm{MLP}(X)$
- Reduce: $X' = SX$
- Connect: $A' = SAS^\top$
- MinCut loss: $\mathcal{L}_c = -\frac{Tr(SAS^\top)}{Tr(SDS^\top)}$
- Orthogonality loss:

$$\mathcal{L}_o = \left\| \frac{SS^\top}{\|SS^\top\|_F} - \frac{I_K}{\sqrt{K}} \right\|_F$$



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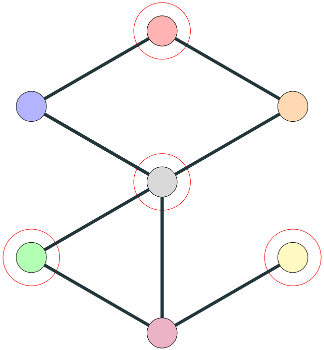
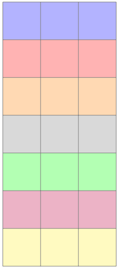
Problem: computing S with neural network is likely to yield a very **dense** matrix.

Can we learn a sparse selection?

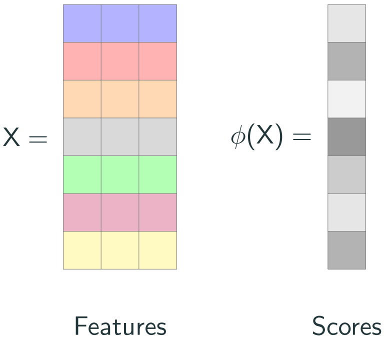


Top-K methods

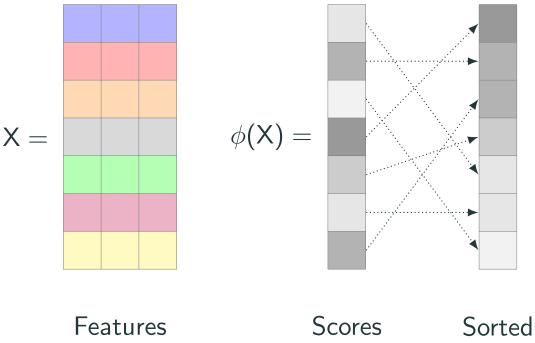
$X =$ 

Features

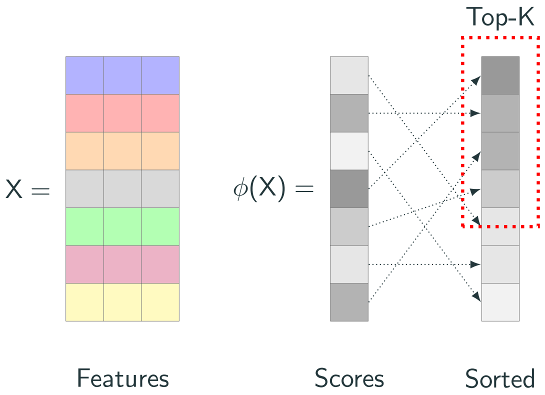
Top-K methods



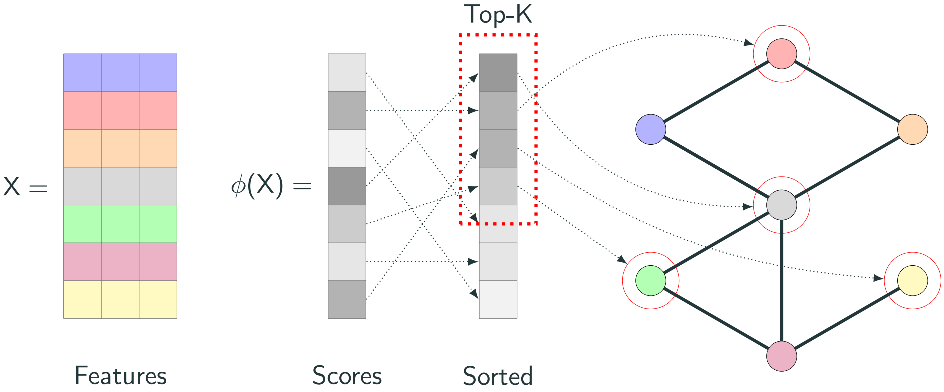
Top-K methods



Top-K methods



Top-K methods



Top-K methods

Different ways of computing the selection indices i:

- Select with a simple linear projection $\theta \in \mathbb{R}^F$ [15];
- Select with a GNN [16];
- Train the selection with a supervised objective (needs ground truth for which nodes to keep) [17].

[15] S. J. Hongyang Gao, "Graph U-Net," 2019.

[16] J. Lee *et al.*, "Self-Attention Graph Pooling," 2019.

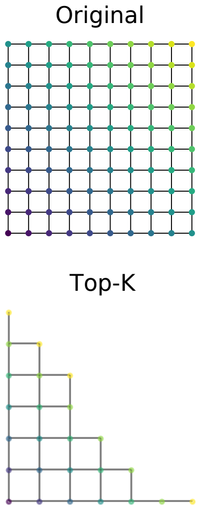
[17] B. Knyazev *et al.*, "Understanding attention in graph neural networks," 2019.

Top-K methods

$$\text{Reduce: } X' = X_i \text{ - Connect: } A' = A_{i,i}$$

Problems:

- Top-k selection is **non-differentiable** (no way of training ϕ). Solved by **gating** (multiplying) the node attributes with the scores.
- Graph is likely to be **disconnected** or simply **cut off** (like in the image on the right). Not really solvable...



Main properties of pooling operators

- **Dense vs. Sparse**: how many nodes are selected for the supernodes (O(N) vs. O(1));
- **Fixed vs. Adaptive**: how many supernodes does the selection compute (*e.g.*, DiffPool/MinCut are fixed);
- **Model-free vs. Model-based**: learn to pool from data or based on a *model* of how to pool;

Global pooling

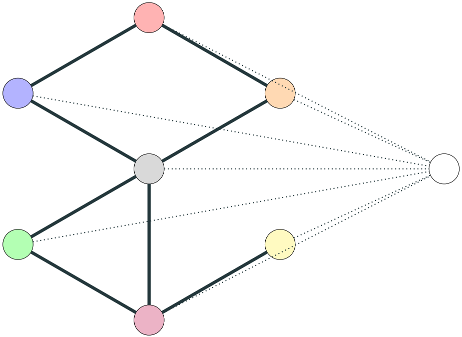
Global Pooling

In CNNs, after convolution, we usually **flatten** out the images to give a vector as input to a MLP:

1	2	3
4	5	6
7	8	9

1	2	3	4	5	6	7	8	9

The graph equivalent must be **invariant to permutations** of the nodes:



Global Pooling

Once again, there are many ways to do this:

- Sum, average, product, max;
- Weighted sum with attention [18];
- Sum and then apply a neural network [19];

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[18] Y. Li *et al.*, "Gated graph sequence neural networks," 2015.

[19] N. Navarin *et al.*, "Universal readout for graph convolutional neural networks," 2019.

Open questions

- Does pooling really work? [20]
    - Which task benefit from it, *a priori*?
- Can we make a pooling layer that is dense, model-free, and adaptive?

[20] D. Mesquita *et al.*, "Rethinking pooling in graph neural networks," 2020.

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