Università della Svizzera italiana

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Istituto Dalle Molle di studi sull'intelligenza artificiale

IDSIA

Pooling in Graph Neural Networks

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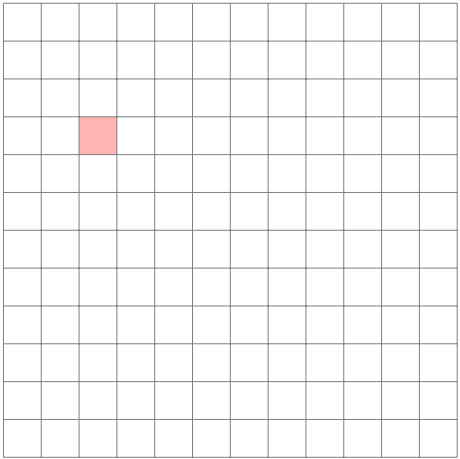
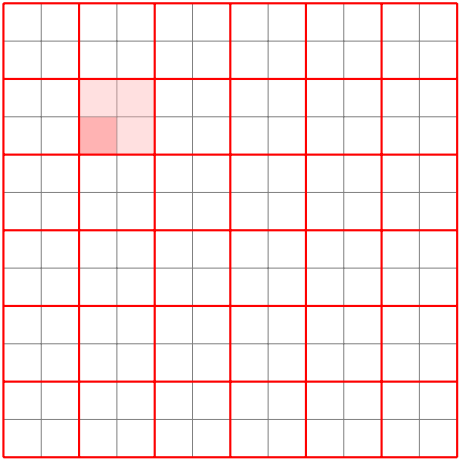
Pooling in CNNs



Pooling in CNNs



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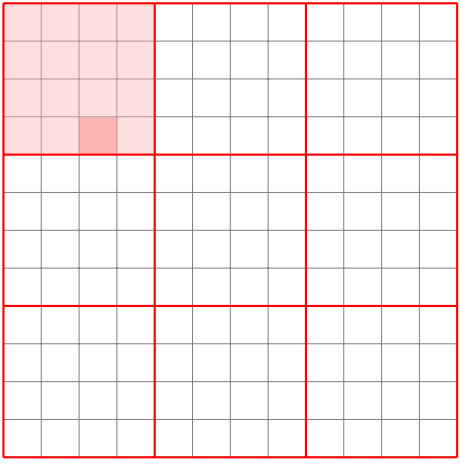

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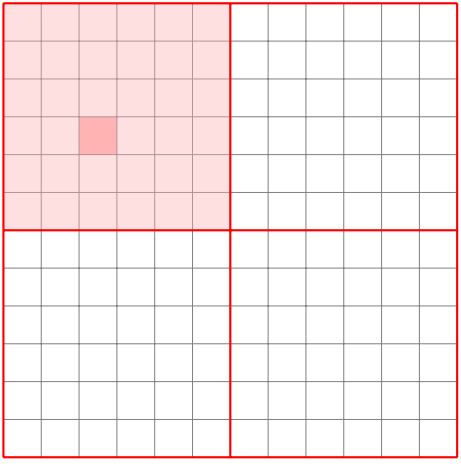

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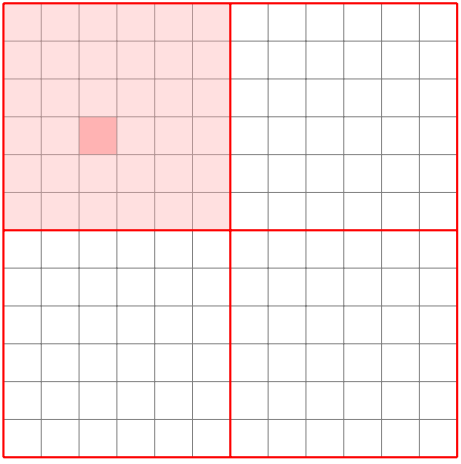

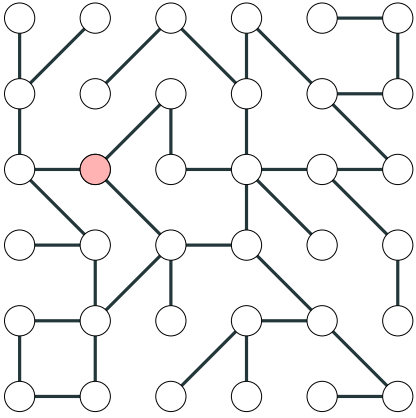

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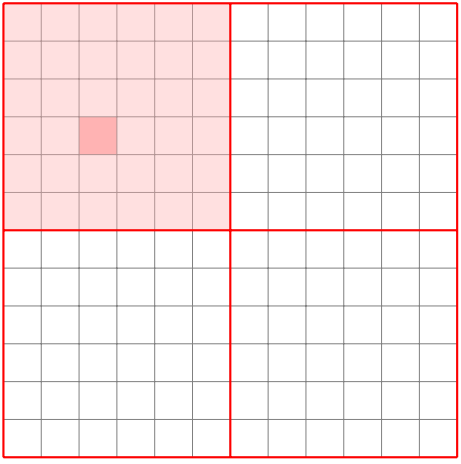

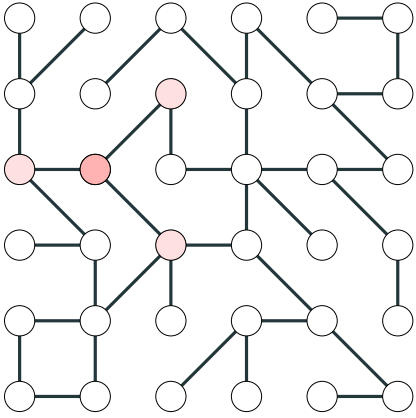

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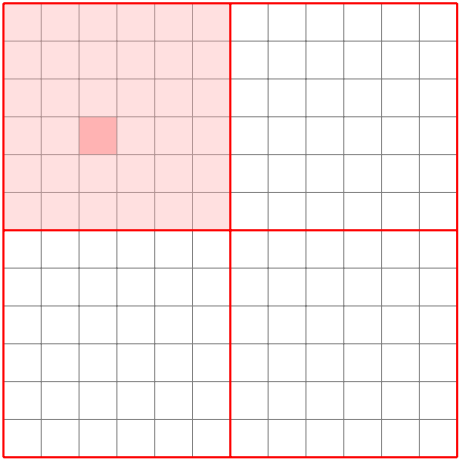

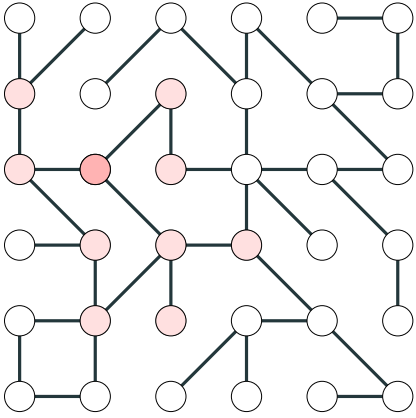

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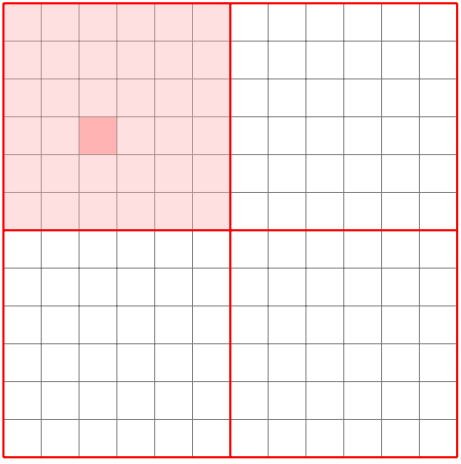
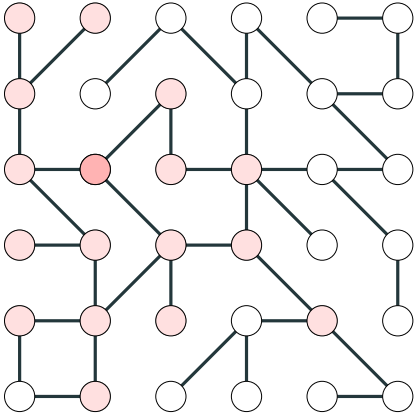




Roadmap

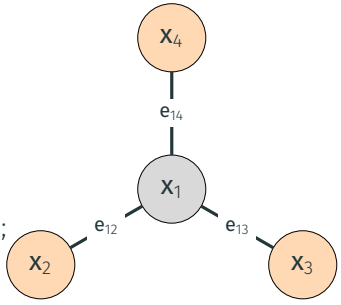
Things we are going to cover:

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

Source: “Understanding pooling in graph neural networks”, Grattarola et al., 2021
https://arxiv.org/abs/2110.05292

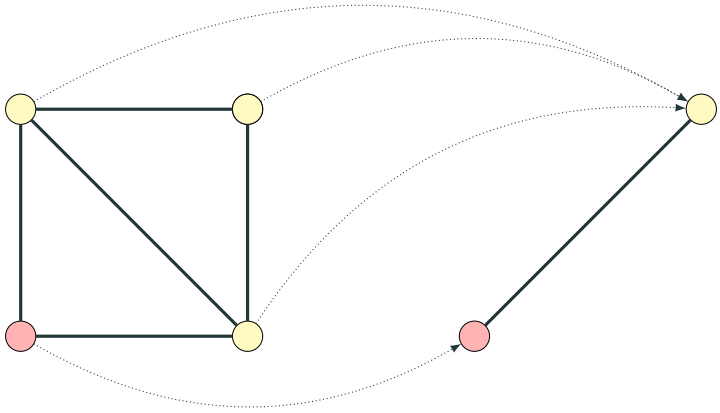
Notation

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



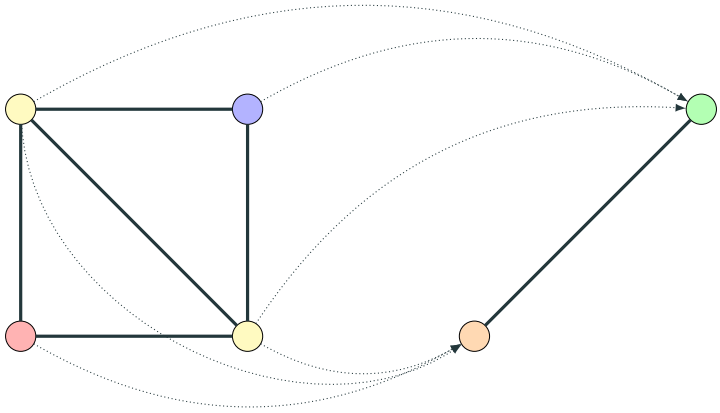
Graph pooling by example

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



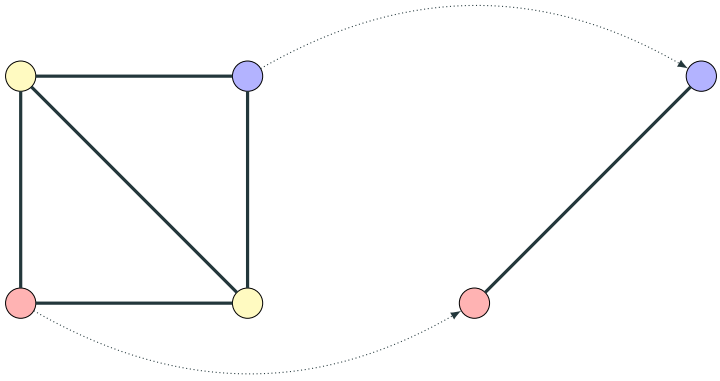
Graph pooling by example

Strategy 2: aggregate cliques.



Graph pooling by example

Strategy 3: keep only some types/colors.



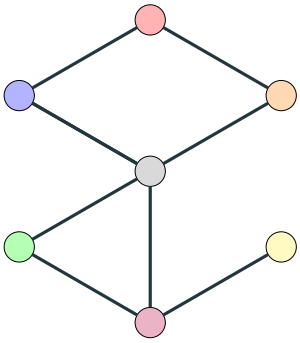
Three main questions [1]

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?

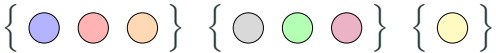
[1] D. Grattarola *et al.*, "Understanding Pooling in Graph Neural Networks," 2021 (In preparation).

Step 1: Select

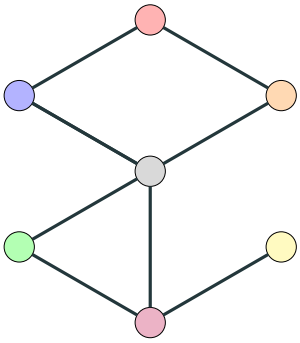
Selecting nodes



Example 1: partition.



Selecting nodes



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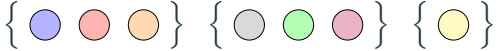
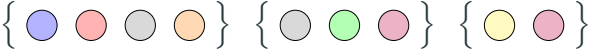
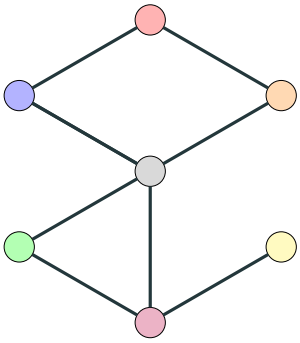


Example 2: cover (possible overlaps).



Selecting nodes



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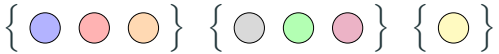
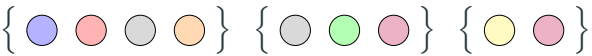


Example 2: cover (possible overlaps).

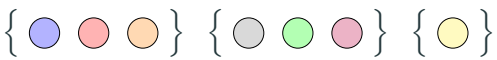


Example 3: sparse.

Selecting nodes

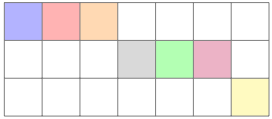
The **selection** stage computes K **supernodes**:

$$\textsc{Sel} : \mathcal{G} \mapsto \mathcal{S} = \{\mathcal{S}_1, \ldots, \mathcal{S}_K\}.$$

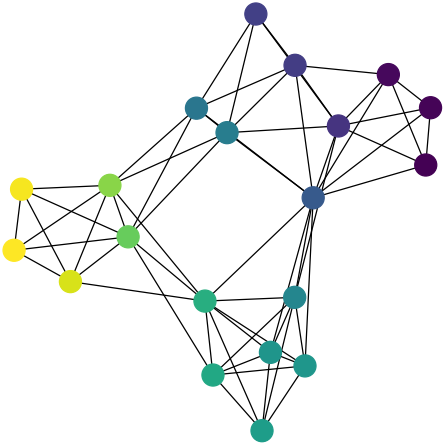


Each supernode is a set of nodes associated with a score:

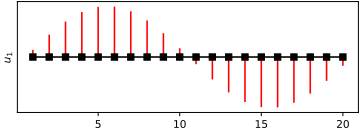
$$\mathcal{S}_k = \{(\mathbf{x}_i, \mathbf{s}_i) \mid \mathbf{s}_i \in \mathbb{R}_{>0}\},$$

$\mathbf{S} =$  $\in \mathbb{R}^{K \times N}$

Spectral clustering [3]



The low-frequency eigenvectors naturally cluster the nodes.

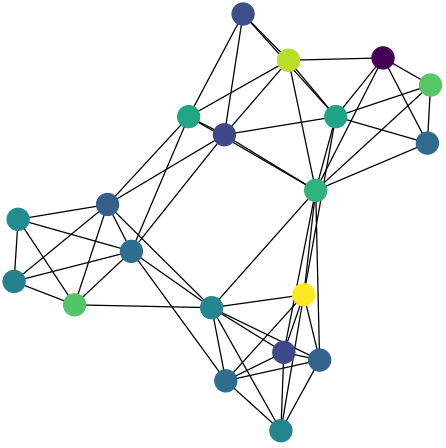


Idea: run k-means clustering (or similar) using the first few eigenvectors.

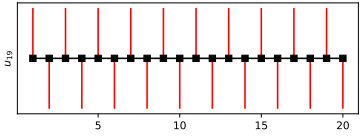
[2] J. Shi *et al.*, "Normalized cuts and image segmentation," 2000.

[3] U. Von Luxburg, "A tutorial on spectral clustering," 2007.

Node decimation [5]



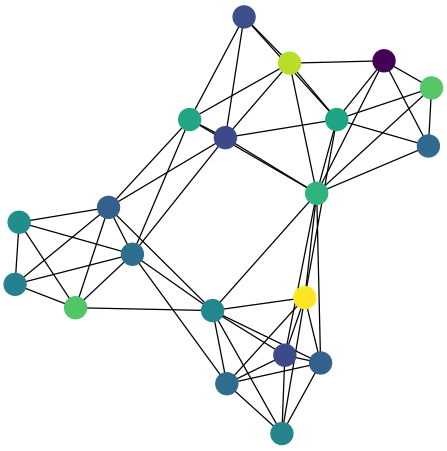
Alternative: use the highest-frequency eigenvector to do something similar to a regular subsampling.



[4] L. Palagi *et al.*, "Computational approaches to max-cut," 2012.

[5] F. M. Bianchi *et al.*, *Hierarchical Representation Learning in Graph Neural Networks with Node Decimation Pooling*, 2019.

Some problems



Problems with spectral methods:

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

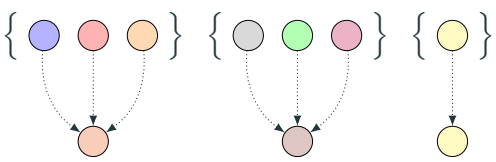
But we get the general idea...

Step 2: Reduce

Reducing supernodes

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

$$\textsc{Red} : \mathcal{G}, \mathcal{S}_k \mapsto \mathbf{x}'_k$$



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

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

Step 3: Connect

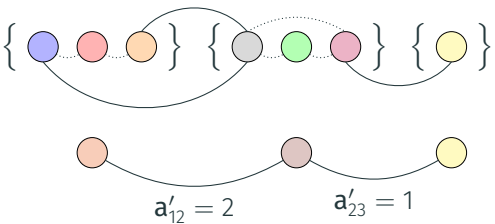
Connecting supernodes

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

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

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

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



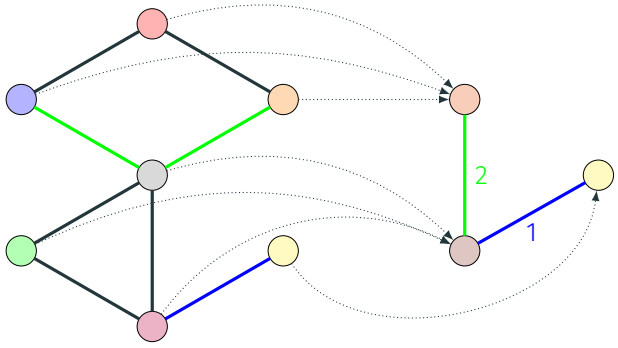
Select, Reduce, Connect [1]

Putting everything together:

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

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

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



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

Methods

Pooling methods

A few ideas:

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

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[8] E. Luzhnica *et al.*, "Clique pooling for graph classification," 2019.

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2. **Clique Pooling** [8]: merge together cliques.
3. **LaPool** [9]: select "leaders" that have higher local variation $\|\mathbf{LX}\|$ w.r.t. all their neighbors. Create clusters by assigning nodes to nearest leader.

[6] I. S. Dhillon *et al.*, "Weighted graph cuts without eigenvectors a multilevel approach," 2007.

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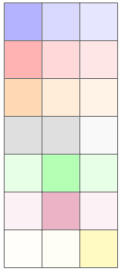
Learning to pool

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

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

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



[10] R. Ying *et al.*, "Hierarchical Graph Representation Learning with Differentiable Pooling," 2018.

[11] F. M. Bianchi *et al.*, "Mincut pooling in Graph Neural Networks," 2019.

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

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- **MinCutPool** [11]: MLP for $\mathbf{S}^\top$, regularize with "minimum cut" loss (same objective as spectral clustering);

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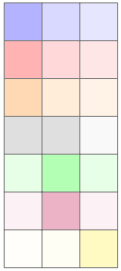

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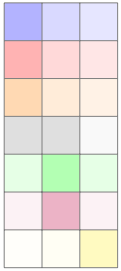
- **MinCutPool** [11]: MLP for $\mathbf{S}^\top$, regularize with "minimum cut" loss (same objective as spectral clustering);
- **Deep Graph Mapper** [12]: combine Mapper [13] and GCN [14] to compute clusters.

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



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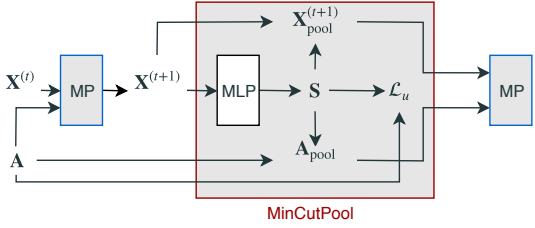
MinCut Pooling [11]

- Select: $\mathbf{S}^\top = \text{MLP}(\mathbf{X})$
- Reduce: $\mathbf{X}' = \mathbf{SX}$
- Connect: $\mathbf{A}' = \mathbf{SAS}^\top$
- MinCut loss: $\mathcal{L}_c = -\frac{Tr(\mathbf{SAS}^\top)}{Tr(\mathbf{SDS}^\top)}$
- Orthogonality loss:
$$\mathcal{L}_o = \left\| \frac{\mathbf{SS}^\top}{\|\mathbf{SS}^\top\|_F} - \frac{\mathbf{I}_K}{\sqrt{K}} \right\|_F$$

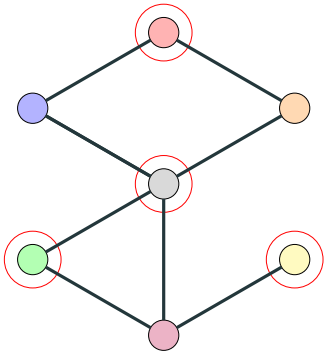


[11] F. M. Bianchi *et al.*, "Mincut pooling in Graph Neural Networks," 2019.

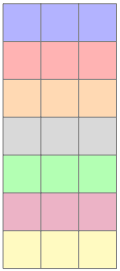
Top-K methods

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

Can we learn a sparse selection?

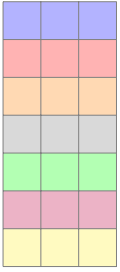


Top-K methods

$X =$ 

Features

Top-K methods

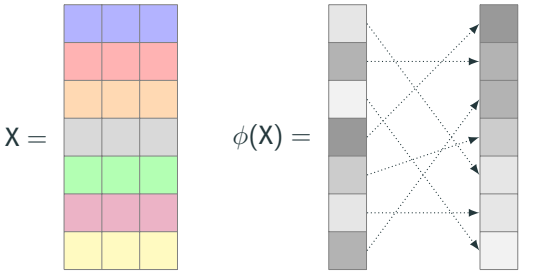
$\mathbf{X} =$ 

Features

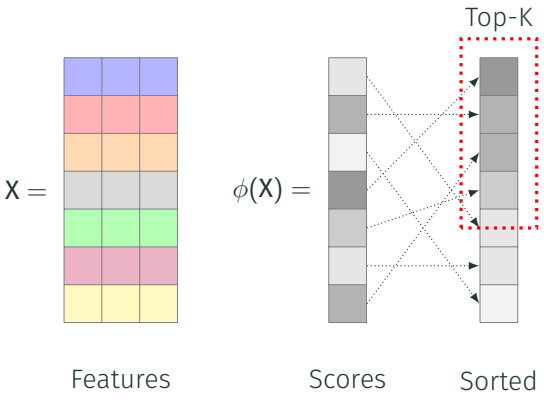
$\phi(\mathbf{X}) =$ 

Scores

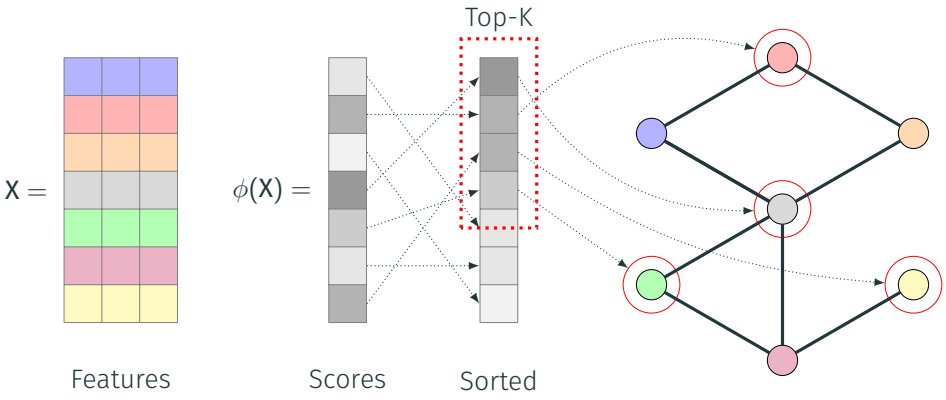
Top-K methods



Top-K methods



Top-K methods



Top-K methods

Different ways of computing the selection indices $\mathbf{i}$:

- 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.

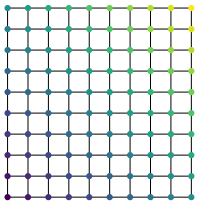
Top-K methods

Reduce: $\mathbf{X}' = \mathbf{X}_i$ - Connect: $\mathbf{A}' = \mathbf{A}_{i,i}$

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...

Original



Top-K

Main properties of pooling operators

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- **Dense vs. Sparse**: how many nodes are selected for the supernodes;
- **Fixed vs. Adaptive**: how many supernodes does the selection compute;
- **Trainable vs. Non-trainable**: learn to pool from data or not;

Global pooling

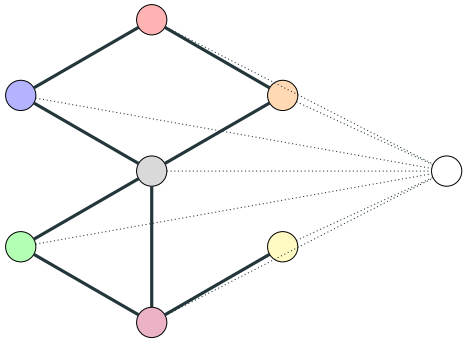
Global Pooling

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;

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

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

Global Pooling

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- Sum, average, product, max;
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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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[19] N. Navarin *et al.*, "Universal readout for graph convolutional neural networks," 2019.

Open questions

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- Does pooling really work?
  - Dense selection + message passing + small graphs is a bad idea [20]

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Open questions

- Does pooling really work?
  - Dense selection + message passing + small graphs is a bad idea [20]
  - Which tasks benefit from pooling *a priori*?
  - Problems with inherent hierarchy?
- Can we make a pooling layer that is dense, trainable, and adaptive?

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References i

[1] D. Grattarola, D. Zambon, F. M. Bianchi, and C. Alippi, "Understanding pooling in graph neural networks,", 2021 (In preparation).

[2] J. Shi and J. Malik, "Normalized cuts and image segmentation," *IEEE Transactions on pattern analysis and machine intelligence*, vol. 22, no. 8, pp. 888–905, 2000.

[3] U. Von Luxburg, "A tutorial on spectral clustering," *Statistics and computing*, vol. 17, no. 4, pp. 395–416, 2007.

[4] L. Palagi, V. Piccialli, F. Rendl, G. Rinaldi, and A. Wiegele, "Computational approaches to max-cut," in *Handbook on semidefinite, conic and polynomial optimization*, Springer, 2012, pp. 821–847.

[5] F. M. Bianchi, D. Grattarola, L. Livi, and C. Alippi, *Hierarchical representation learning in graph neural networks with node decimation pooling*, 2019. arXiv: *1910.11436 [cs.LG]*.

References ii

[6] I. S. Dhillon, Y. Guan, and B. Kulis, "Weighted graph cuts without eigenvectors a multilevel approach," *IEEE transactions on pattern analysis and machine intelligence*, vol. 29, no. 11, pp. 1944–1957, 2007.

[7] M. Defferrard, X. Bresson, and P. Vandergheynst, "Convolutional neural networks on graphs with fast localized spectral filtering," in *Advances in Neural Information Processing Systems*, 2016, pp. 3844–3852.

[8] E. Luzhnica, B. Day, and P. Lio, "Clique pooling for graph classification," *International Conference of Learning Representations (ICLR) – Representation Learning on Graphs and Manifolds workshop*, 2019.

[9] E. Noutahi, D. Beani, J. Horwood, and P. Tossou, "Towards interpretable sparse graph representation learning with laplacian pooling," *arXiv preprint arXiv:1905.11577*, 2019.

References iii

[10] R. Ying, J. You, C. Morris, X. Ren, W. L. Hamilton, and J. Leskovec, "Hierarchical graph representation learning with differentiable pooling," *arXiv preprint arXiv:1806.08804*, 2018.

[11] F. M. Bianchi, D. Grattarola, and C. Alippi, "Mincut pooling in graph neural networks," *CoRR*, vol. abs/1907.00481, 2019. arXiv: *1907.00481*. [Online]. Available: *http://arxiv.org/abs/1907.00481*.

[12] C. Bodnar, C. Cangea, and P. Liò, "Deep graph mapper: Seeing graphs through the neural lens," *arXiv preprint arXiv:2002.03864*, 2020.

[13] G. Singh, F. Mémoli, and G. E. Carlsson, "Topological methods for the analysis of high dimensional data sets and 3d object recognition.," in *SPBG*, 2007, pp. 91–100.

[14] T. N. Kipf and M. Welling, "Semi-supervised classification with graph convolutional networks," in *International Conference on Learning Representations (ICLR)*, 2016.

References iv

[15] S. J. Hongyang Gao, "Graph u-net," *Submitted to ICLR*, 2019.

[16] J. Lee, I. Lee, and J. Kang, "Self-attention graph pooling," *arXiv preprint arXiv:1904.08082*, 2019.

[17] B. Knyazev, G. W. Taylor, and M. R. Amer, "Understanding attention in graph neural networks," *CoRR*, vol. abs/1905.02850, 2019. arXiv: *1905.02850*. [Online]. Available: *http://arxiv.org/abs/1905.02850*.

[18] Y. Li, D. Tarlow, M. Brockschmidt, and R. Zemel, "Gated graph sequence neural networks," *arXiv preprint arXiv:1511.05493*, 2015.

[19] N. Navarin, D. Van Tran, and A. Sperduti, "Universal readout for graph convolutional neural networks," in *2019 International Joint Conference on Neural Networks (IJCNN)*, IEEE, 2019, pp. 1–7.

[20] D. Mesquita, A. Souza, and S. Kaski, “Rethinking pooling in graph neural networks,” *Advances in Neural Information Processing Systems*, vol. 33, 2020.