



Graph Pooling: DIFFPOOL

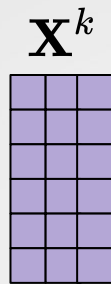
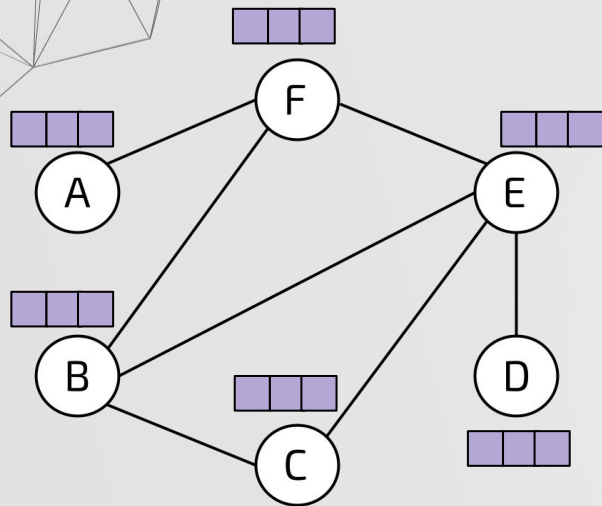
Giovanni Pellegrini^{1,2,3}

SML¹ Lab, University of Trento, Italy

TIM²

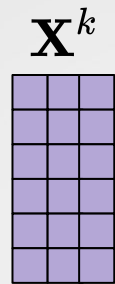
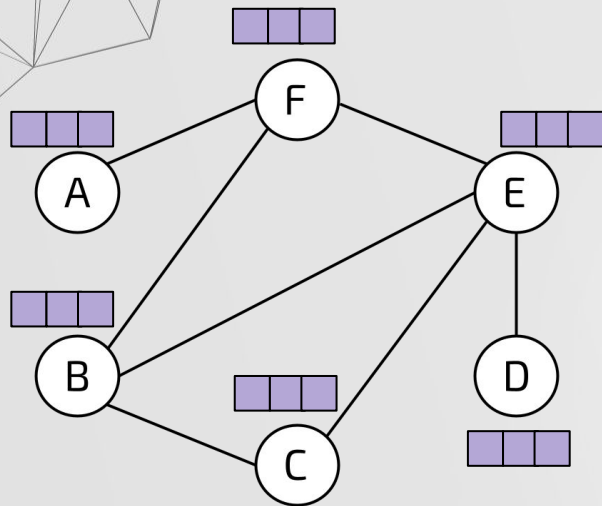
EIT DIGITAL³

01 Graph prediction



$$\mathbf{X}^{t+1} = \text{GConv}(\mathbf{A}, \mathbf{X}^t, \mathbf{W}^t) \quad t = 1, \dots, k$$

01 Graph prediction



$GPool(\mathbf{X}^k)$

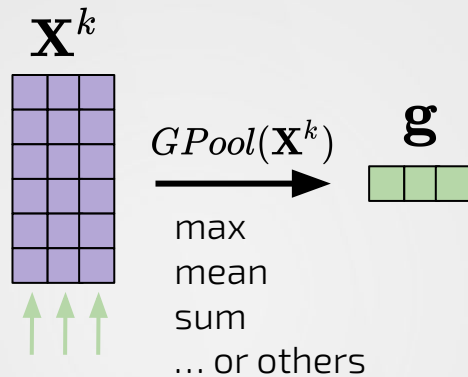
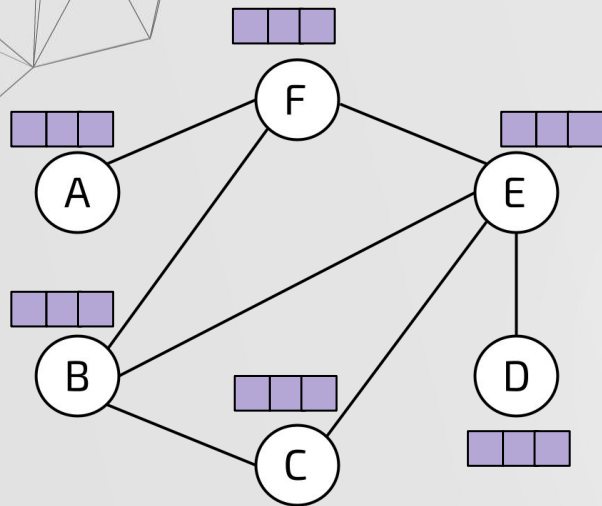


max
mean
sum
... or others

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$GPool(\mathbf{X}^k) \longrightarrow$ global pooling function

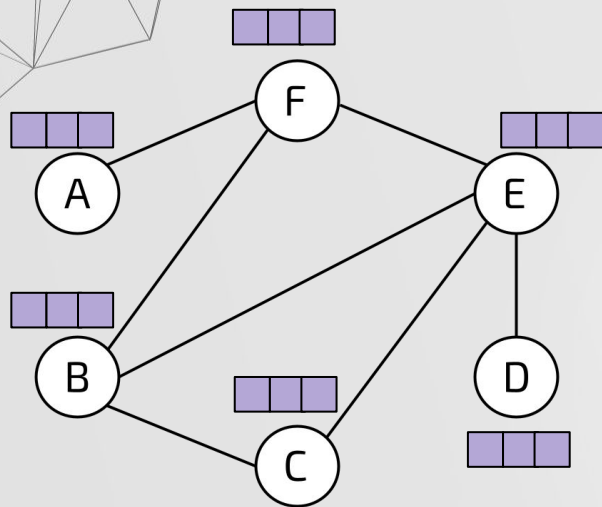
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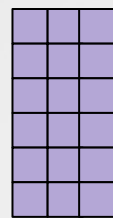
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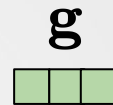


\mathbf{X}^k



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$O(\mathbf{W}, \mathbf{g})$



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$GPool(\mathbf{X}^k) \longrightarrow$ global pooling function

$O(\mathbf{W}, \mathbf{g}) \longrightarrow$ graph readout function



01 Graph prediction

Equivalent to having a virtual “supernode” in the last layer connected to all the nodes in the graph

Pooling the node embeddings all together do not capture hierarchical representations of the network



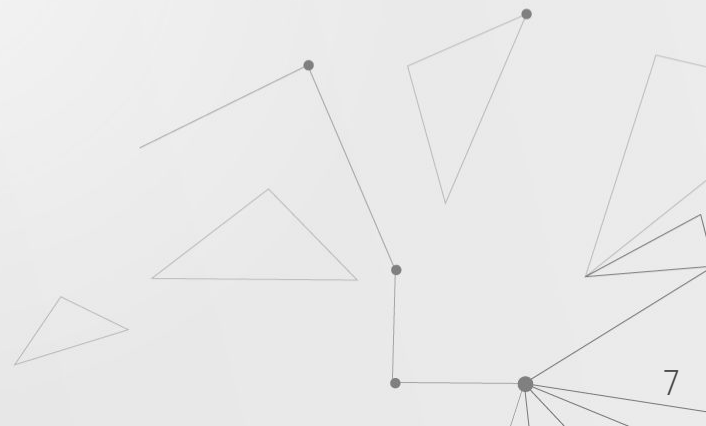


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DIFFPOOL: hierarchical nodes pooling strategy





02 DIFFPOOL¹

DIFFerentiable **POOL**ing: Compute an hierarchical representation of the graph by aggregating “close” nodes

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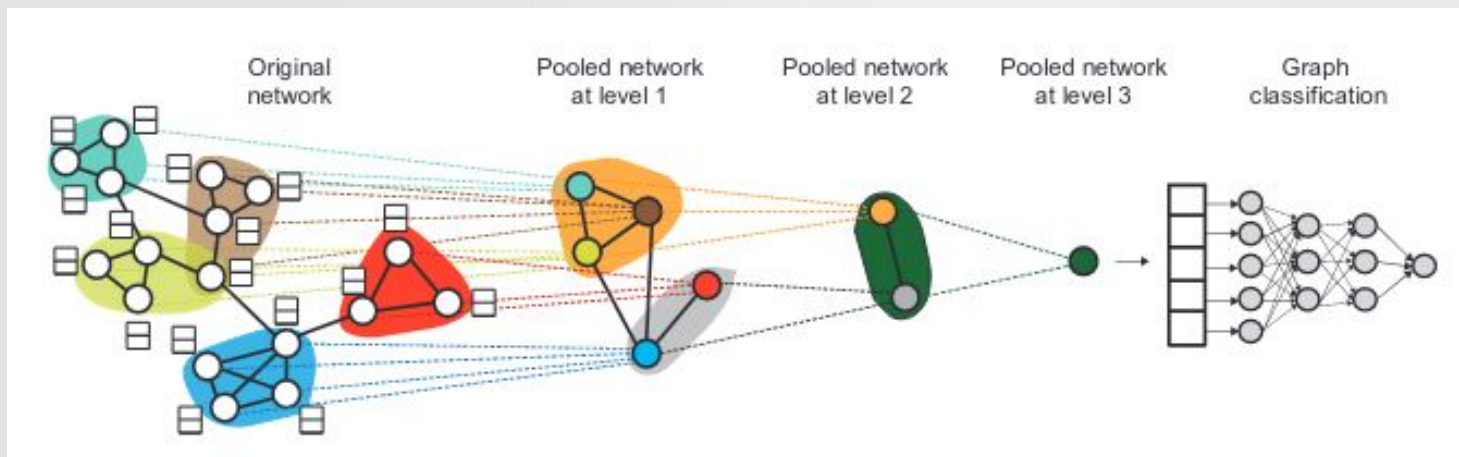


Image taken from the original publication.

02 DIFFPOOL

Idea: stack several GNN and pooling layer on top of each other




\mathbf{A}^0

\mathbf{X}^0



02 DIFFPOOL


$$G = (A, X)$$

adjacency
matrix

node features
matrix

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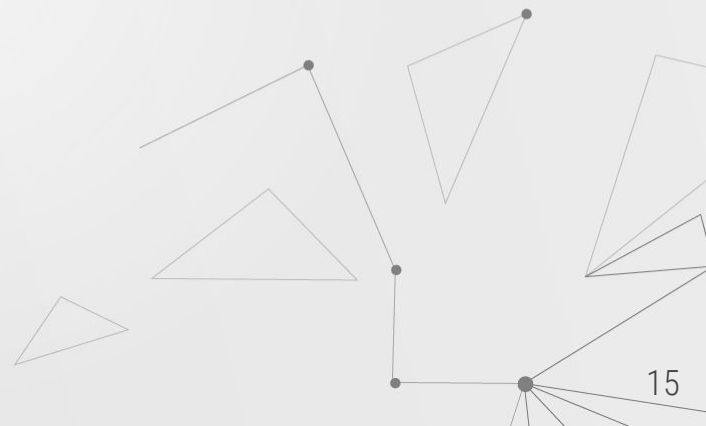
$$\mathbf{Z} = \text{GNN}(\mathbf{A}, \mathbf{X})$$

arbitrary GNN that computes K iterations, $\mathbf{Z} = \mathbf{X}^K$



02 DIFFPOOL

Given **A** and **Z** , find a coarse representation of the graph





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$$\begin{array}{ccc} \mathbf{A} \in R^{n \times n} & \longrightarrow & \mathbf{A}' \in R^{m \times m} \\ \mathbf{Z} = R^{n \times d} & & \mathbf{Z}' = R^{m \times d} \end{array} \quad \text{with } m < n$$

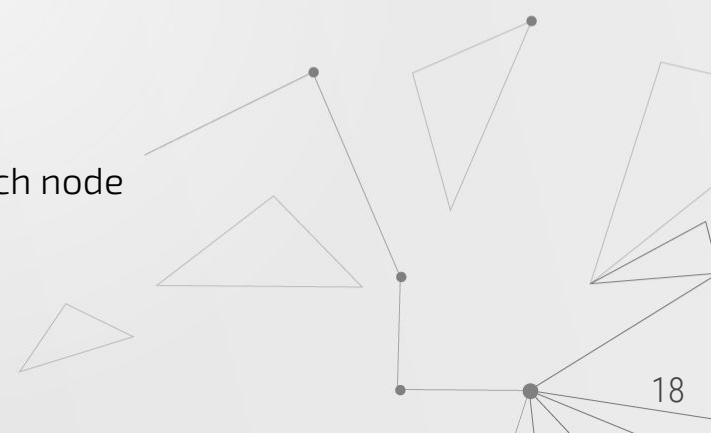


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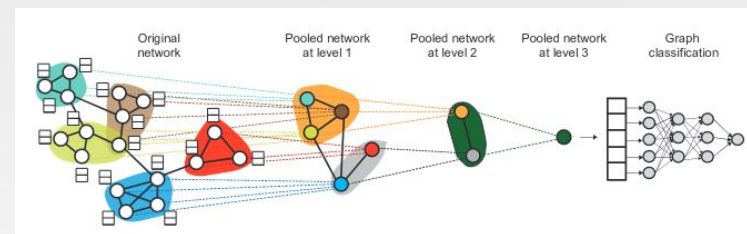
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Solution -> learn a cluster assignment for each node



03 Pooling in DIFFPOOL

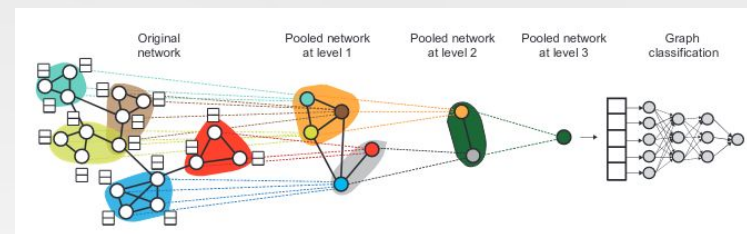
The final representation is obtained by coarsening the graph in L hierarchical steps. To do that, at each step a **cluster assignment matrix** is learned.



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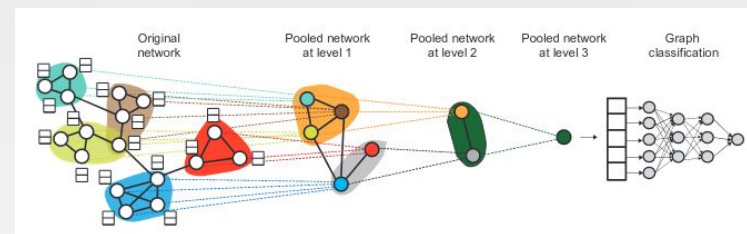
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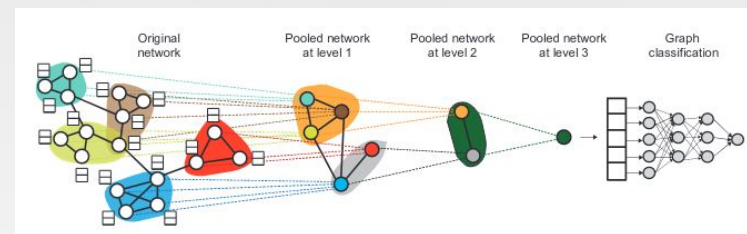
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↗ transposed



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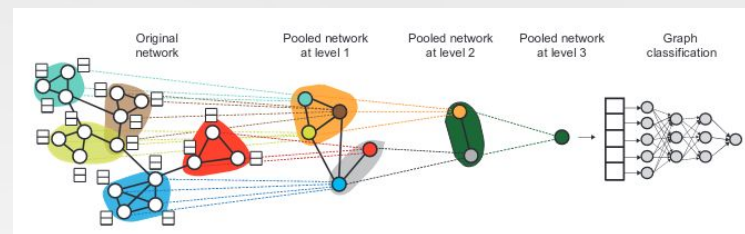
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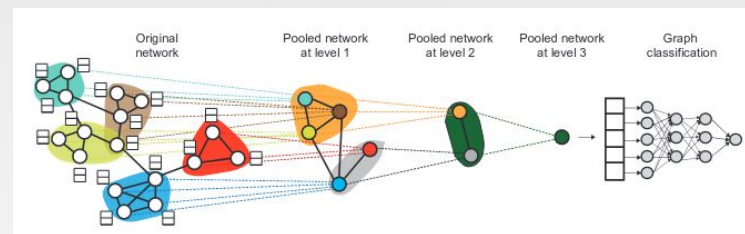
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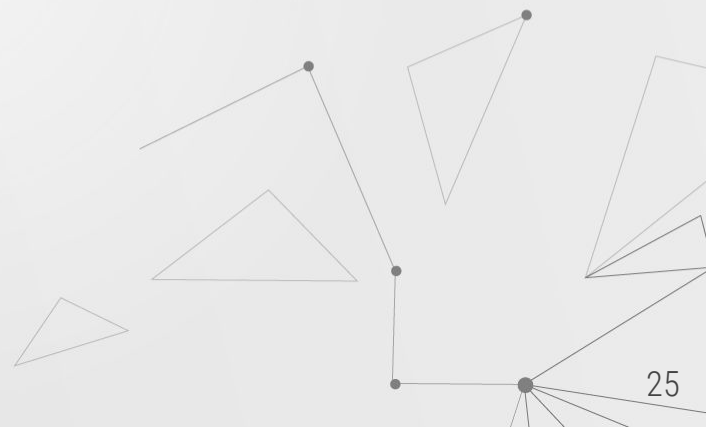


The number of clusters at each step is an hyperparameter!



04 Learning the assignment matrix

How is the cluster matrix learned?

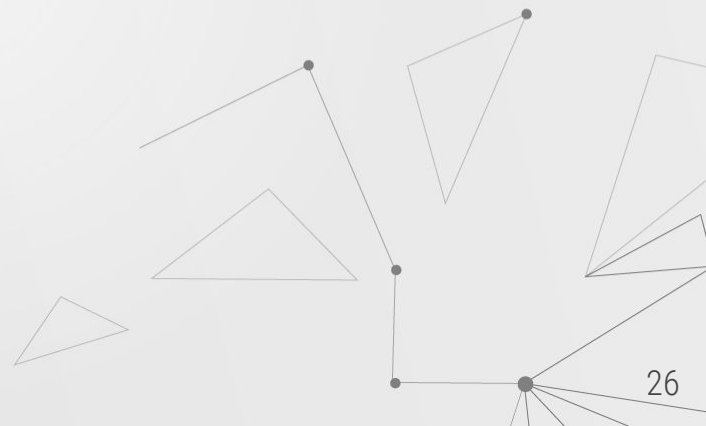




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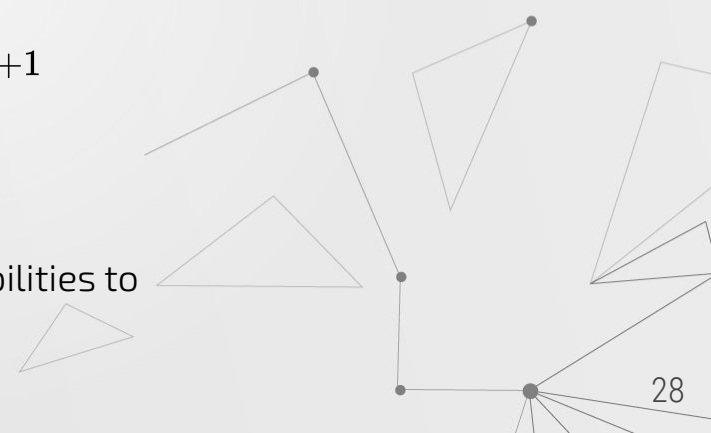
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$$\text{GNN}_{\text{pool}}^l \xrightarrow{\text{outputs}} \mathbf{R}^{n^l \times n^{l+1}}$$

Softmax is applied row-wise, it assigns probabilities to which clusters to belong to in the next step.



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differentiable!

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05 Final prediction

At the last step the graph is condensed in one single node (vector). The final prediction is the output of a MLP.

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Let's switch to the notebook...

