Aggregation Functions in GNNs

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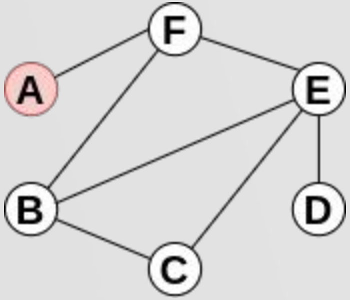
TIM[2]
EIT DIGITAL[3]

COMPUTATION GRAPH

The neighbour of a node defines its computation graph

INPUT GRAPH



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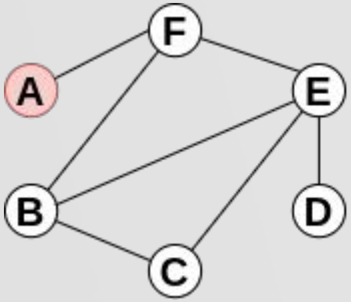

COMPUTATION GRAPH

01 Recap

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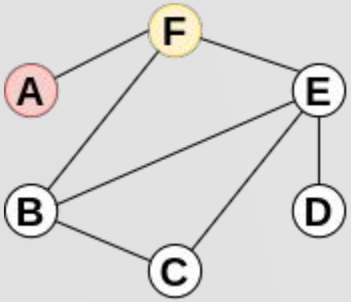

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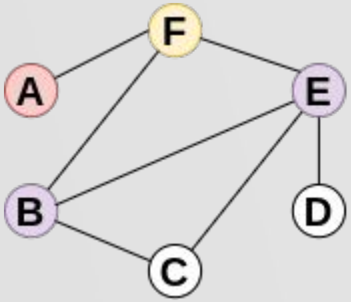

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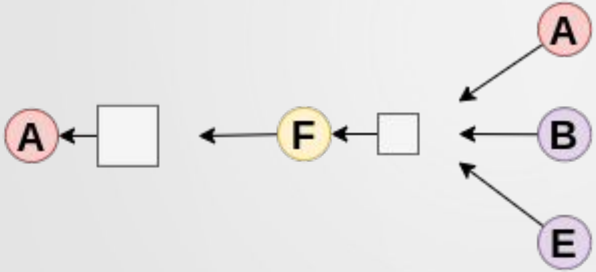

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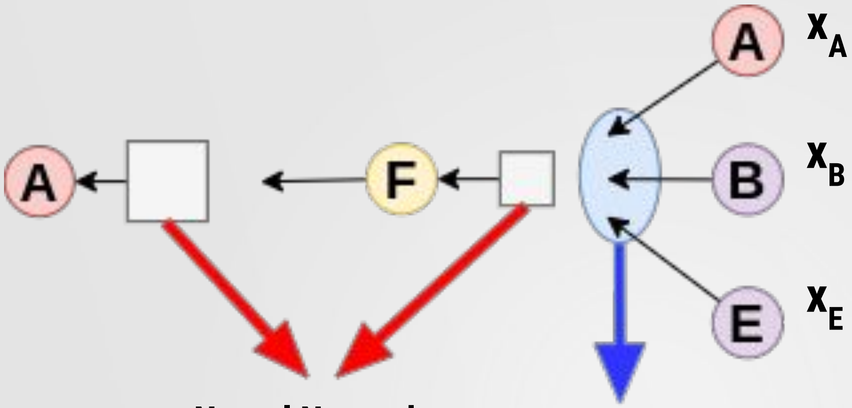


Neural Networks

<u>Permutation invariant</u>
Aggregation

Sum
Average
Max

01 Recap

GCN	mean
GraphSage	max, mean, LSTM
GAT	sum

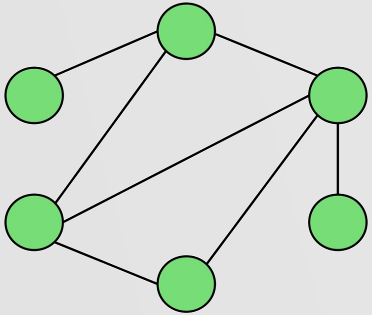
TABLE OF CONTENTS

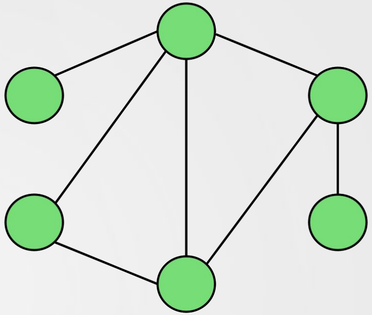
02 WL Isomorphism Test

Solution: Weisfeiler-Lehman isomorphism test[1]

[1] Weisfeiler and Lehman. *A reduction of a graph to a canonical form and an algebra arising during this reduction.* Nauchno-Technicheskaya Informatsia, 1968.

02 WL Isomorphism Test





Step 0

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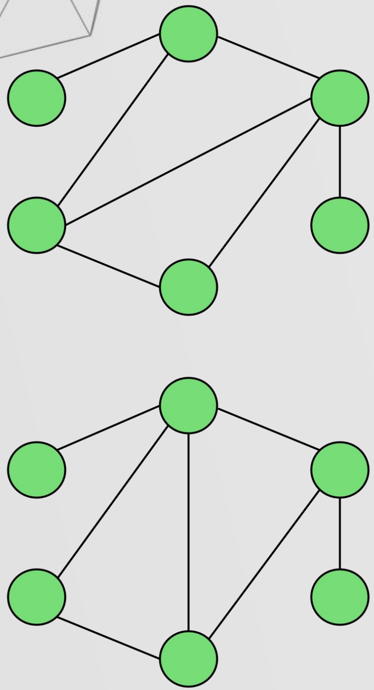

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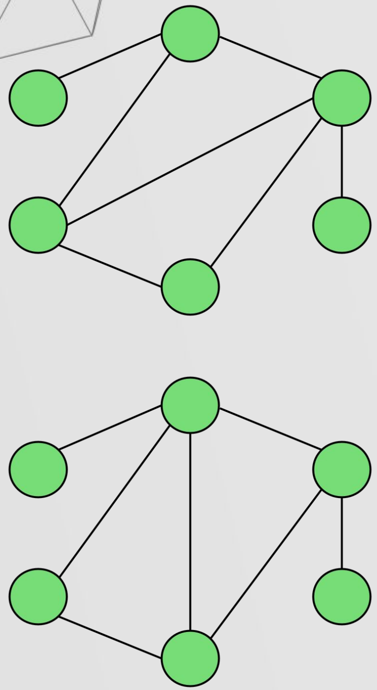

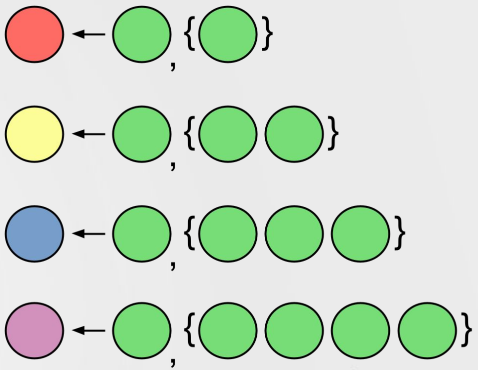

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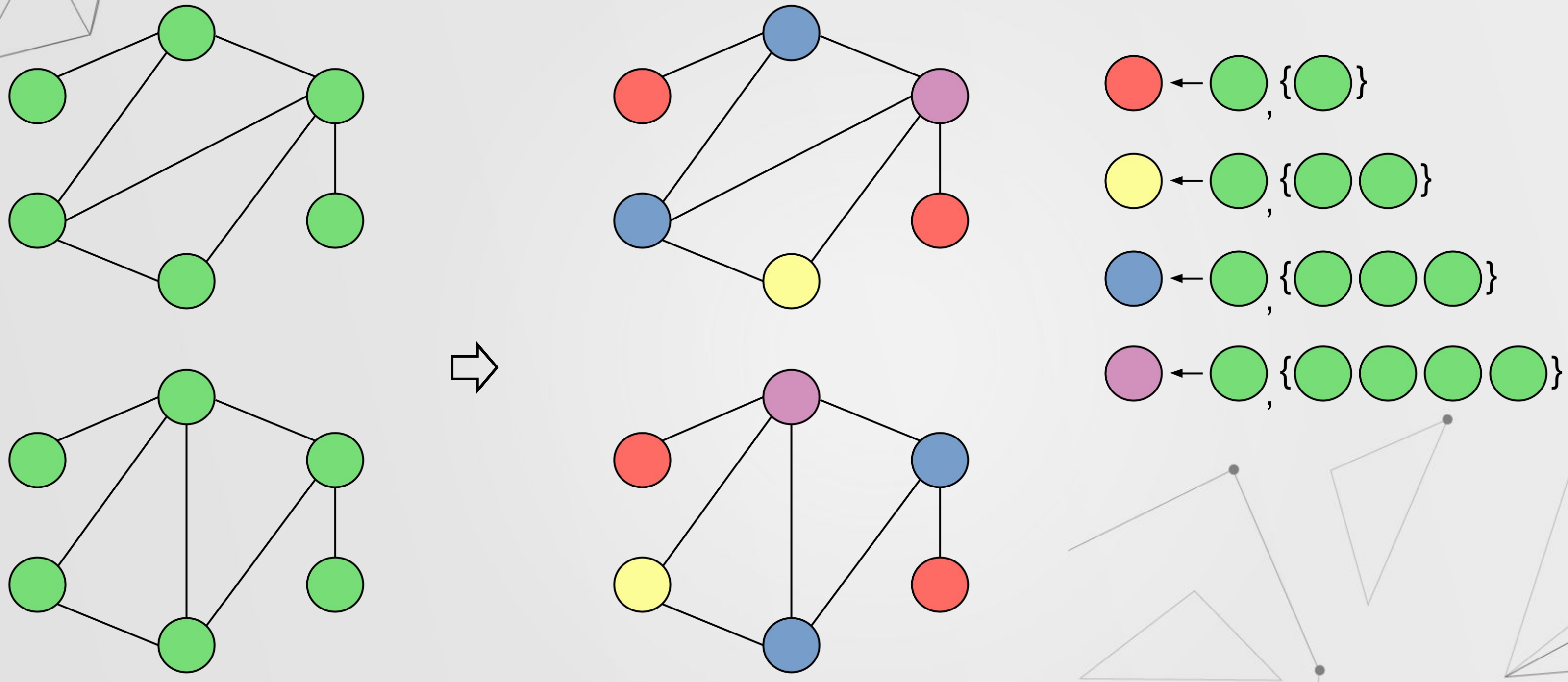

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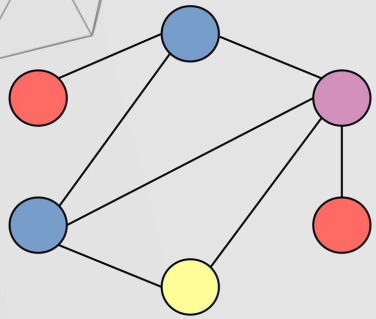

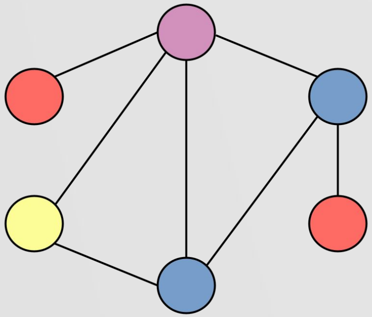

Step 2

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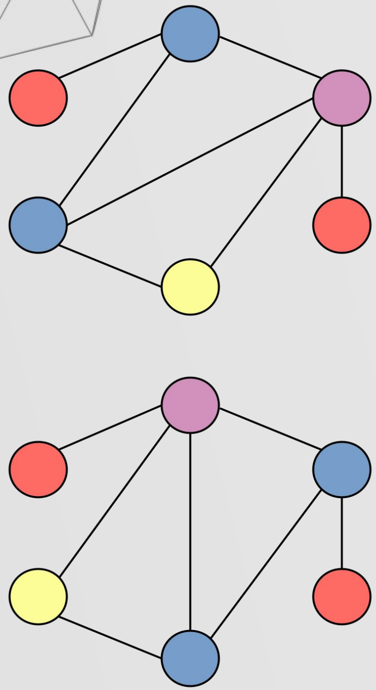

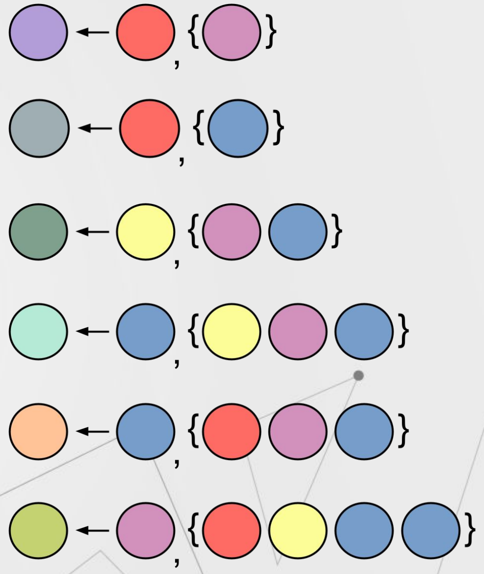

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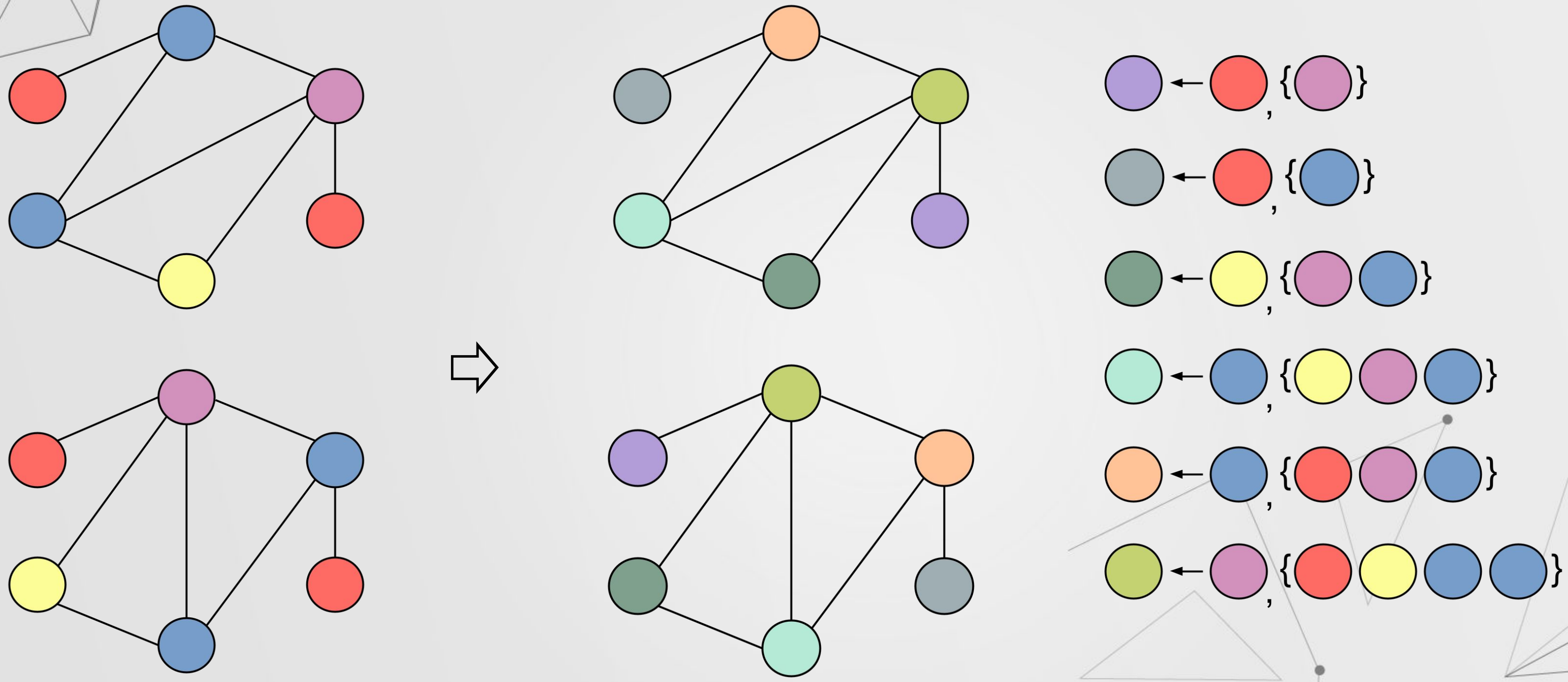

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- Efficient heuristic
- Isomorphic graphs -> same labels
- Nodes are uniquely coloured
- Distinguish most graphs

But… limited use in practice

03 Graph Isomorphism Network (GIN)

Can we construct a GNNs as powerful as the WL isomorphism test?

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GIN - Graph Isomorphism Network[2]

[2] Xu et al., *How powerful are graph neural networks?*, International Conference on Learning Representations, 2019

03 Graph Isomorphism Network (GIN)

G, G' two non-isomorphic graphs

$\mathcal{A} : G \to \mathbb{R}^d$ a GNN

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Sum-decomposition

04 Sum-decomposition[3]

Any injective function on multisets can be decomposed as

$$g(X) = \phi\Big(\sum_{x \in X} f(x)\Big)$$

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Any injective function on multisets can be decomposed as

$$g(X) = \phi\left(\sum_{x \in X} f(x)\right)$$

$$g(\boldsymbol{h}, X) = \phi\Big((1+\epsilon) \cdot f(\boldsymbol{h}) + \sum_{\boldsymbol{x} \in X} f(\boldsymbol{x})\Big)$$

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04 Back to GIN

Use an MLP for representing $\phi \circ f$

$$\boldsymbol{h}_i^{(k)} = \mathrm{MLP}^{(k)}\left(\left(1 + \epsilon^{(k)}\right) \cdot \boldsymbol{h}_i^{(k-1)} + \sum_{j \in \mathcal{N}(i)} \boldsymbol{h}_j^{(k-1)}\right)$$

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Cons of sum-decomposition:

- Highly discontinuous functions
- For uncountable domains, latent dimension of f should be higher than the number of elements in the set[4]
- No guarantee to find the right function

[4]Wagstaff et al., *On the limitations of representing functions on sets*, Proceedings of the 36th International Conference on Machine Learning, 2019

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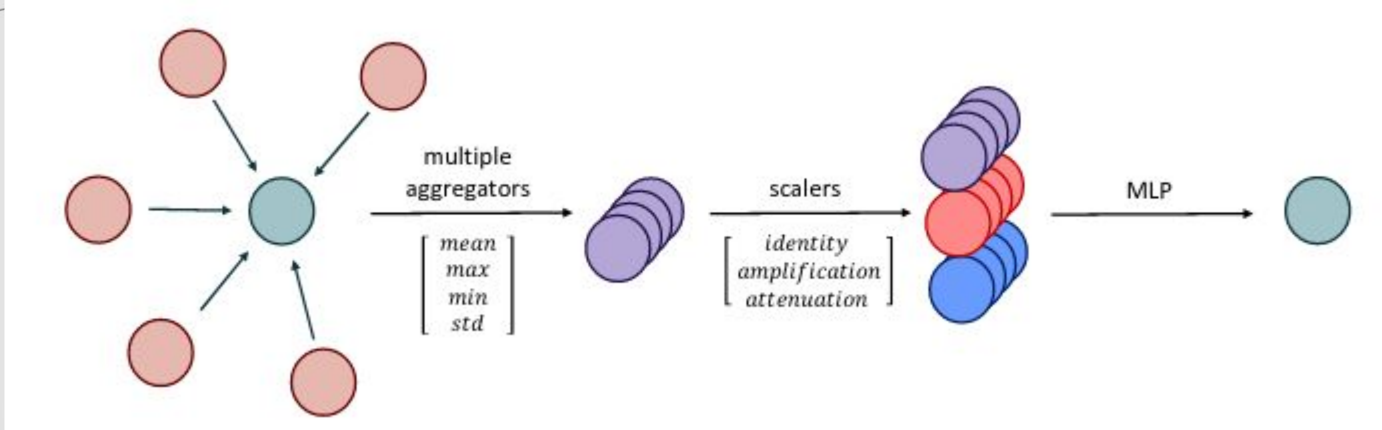

Image taken from the arXiv version of the paper.

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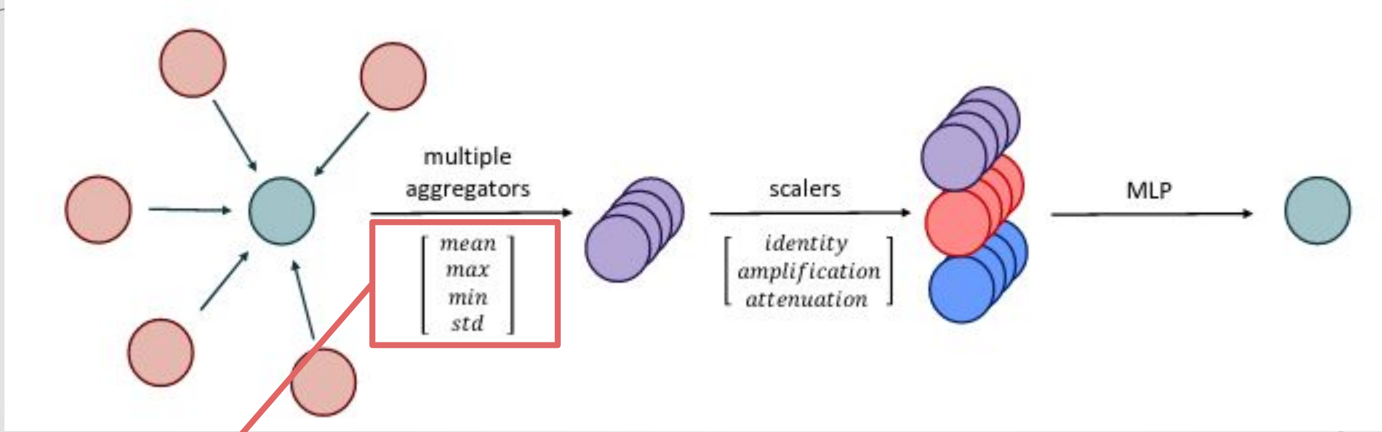

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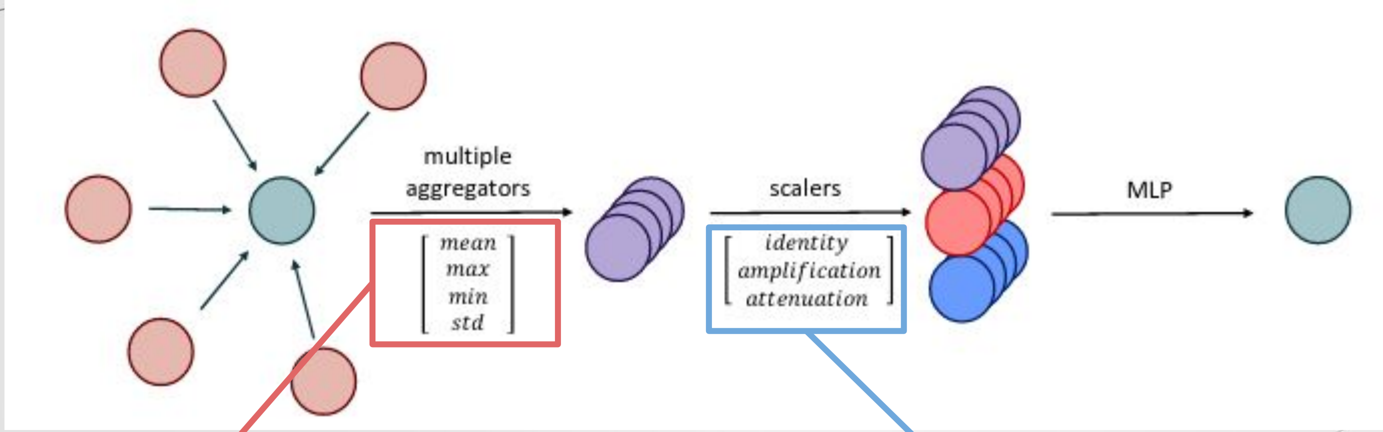

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Library of aggregators

Logarithmic scalers

[5]Corso et al., *Principal Neighbourhood Aggregation for Graph Nets*, Advances in Neural Information Processing Systems 33 (NeurIPS 2020), 2020

05 Principal Neighborhood Aggregation[5]

$$S = \left(\frac{\log(d+1)}{\delta}\right)^{\alpha}$$

$$\delta = \frac{1}{|train|} \sum_{i \in train} \log(d_i + 1)$$

$S_{amp}, \alpha = 1$ $S_{att}, \alpha = -1$ $S_{identity}$

06 Learning Aggregation Functions[6]

Don’t choose the aggregation function(s) - learn it!

[5]Pellegrini et al., *Learning Aggregation Functions*, under revision, 2020

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Learnable parameters

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MAX, MIN, SUM, MEAN, MOMENTS, MIN/MAX, COUNT ...

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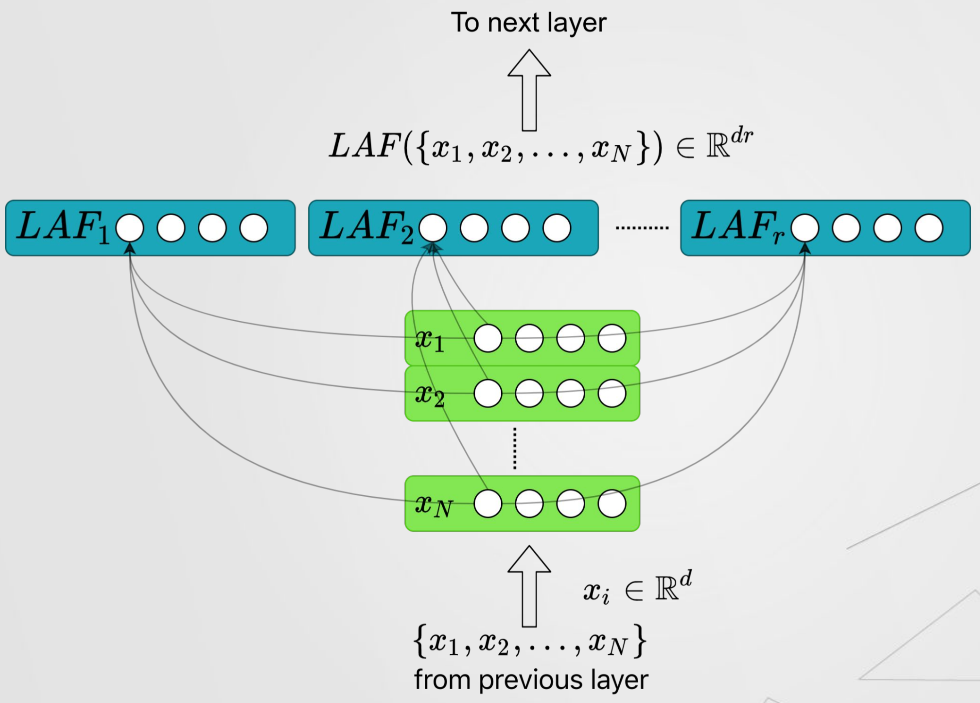

07 Aggregation in Pytorch Geometric

PyTorch Geometric provides the MessagePassing base class.

METHODS

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Aggregates messages from neighbors (sum, mean, max)

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Constructs messages from node j to node i in analogy to ϕΘ

message (**x_j**: torch.Tensor) → **torch.Tensor** [source]

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