Autoregressive Models for Sequences of Graphs

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Sequences of graphs

A **graph** of N nodes is a tuple $g = (\mathcal{V}, \mathcal{E}) \in \mathcal{G}$ s.t.:

$$\mathcal{V} = \{v_i \in \mathbb{R}^F\}_{i=1,\dots,N} \qquad \mathcal{E} = \{e_{ij} \in \mathbb{R}^S\}_{v_i, v_j \in \mathcal{V}}$$

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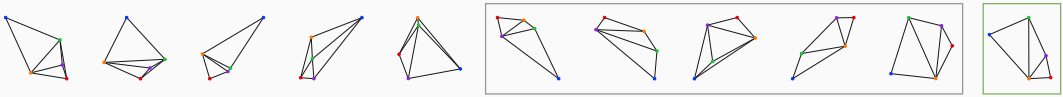

Problem formulation: graph autoregression

Traditional AR model

$$f : \mathbb{R}^{p \times d} \to \mathbb{R}^d$$

$$x_{t+1} = f(\boldsymbol{x}_t^p) + \epsilon$$

$$f(\boldsymbol{x}_t^p) = \mathbb{E}[f(\boldsymbol{x}_t^p) + \epsilon]$$

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Where:

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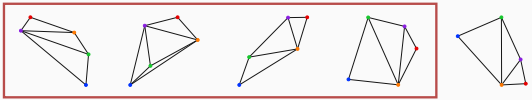
Implementing $\phi(g_t^p)$



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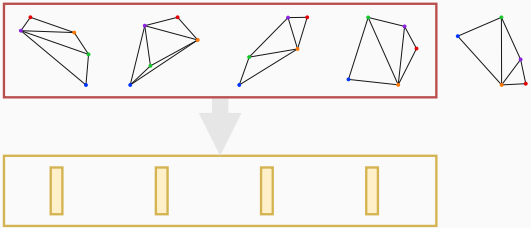
Graph embedding

$\phi_{emb}(\,\cdot\,;\theta_{emb}) : \mathcal{G} \to \mathbb{R}^l$, applied in parallel to each graph in the regressor.



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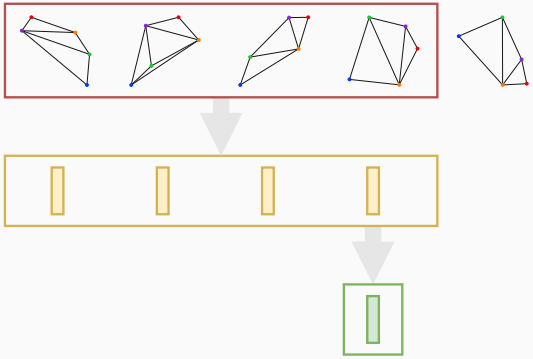
Vector prediction

$\phi_{prd}(\,\cdot\,;\theta_{prd}) : \mathbb{R}^{k\times l} \to \mathbb{R}^l$, captures temporal dynamics in embedding space.



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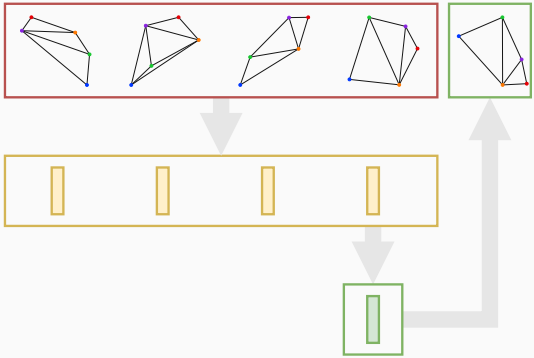
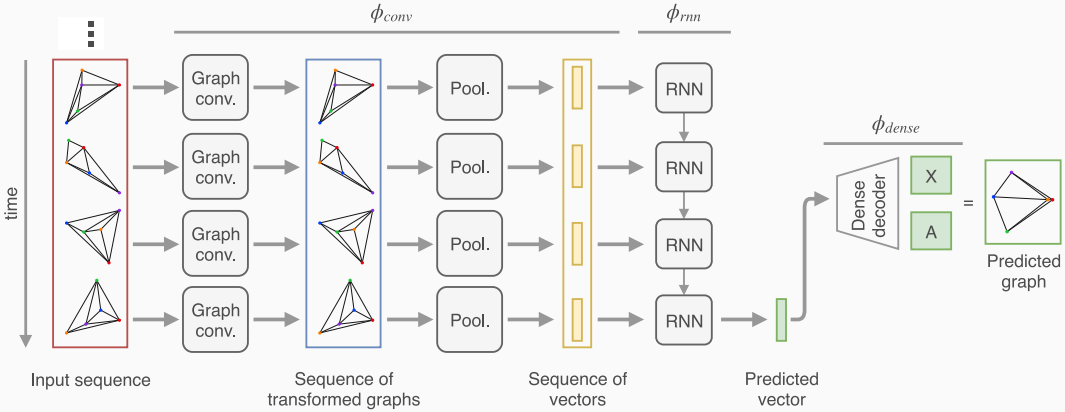
Graph decoder

$\phi_{dec}(\cdot\,;\theta_{dec}) : \mathbb{R}^l \to \mathcal{G}$, outputs graph from predicted vector.



Implementing $\phi(g_t^p)$ with a GNN



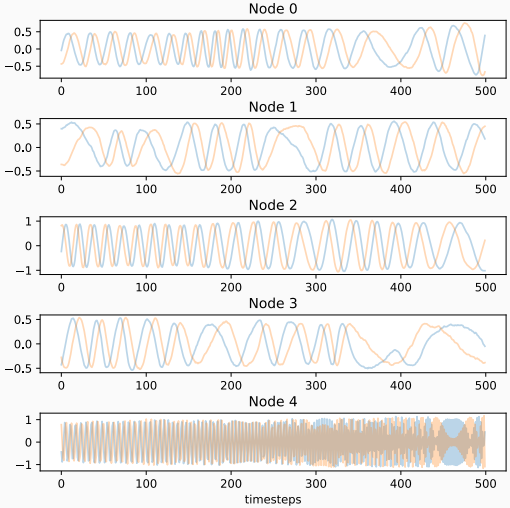
Experiments: rotational model

Points moving in a 2D plane with delayed rotations:

$$f(\boldsymbol{x}_t^p) = R(\boldsymbol{x}_t^p) \cdot x_t$$

$$R_n(\boldsymbol{x}_t^p) = \begin{bmatrix} \cos(\omega) & \sin(\omega) \\ -\sin(\omega) & \cos(\omega) \end{bmatrix}$$

$$\omega = c_n + \alpha \cos\left(\sum_{i=0}^{p-1} x_{t-i,2n-1} + x_{t-i,2n}\right)$$



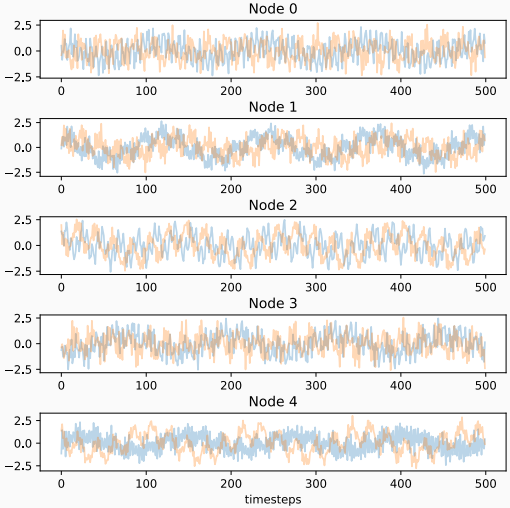
Experiments: Partially Masked Linear Dynamical System (PMLDS)

Given a c-dimensional oscillating linear system:

$$x_{t+1} = Rx_t$$

$$x_t \in \mathbb{R}^c \text{ and } R \in \mathbb{R}^{c \times c}$$

we only observe the top $N \cdot F$ components. This results in a dynamical system of order $p \propto (c - N \cdot F)$ [1].



[1] E. Ott, *Chaos in Dynamical Systems*, 2002.

Baselines

Mean

Assumes GSP is stationary, predicts the mean graph: $\hat{g}_{t+1} = \mathbb{E}^{\mathrm{f}}[g]$.

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Moving average

Predicts the mean graph from the k preceding observations:

$$\hat{g}_{t+1} = \mathbb{E}^{\mathrm{f}}[\boldsymbol{g}_t^k] = \arg\min_{g'} \sum_{g_i \in \boldsymbol{g}_t^k} \mathrm{d}(g', g_i)^2.$$

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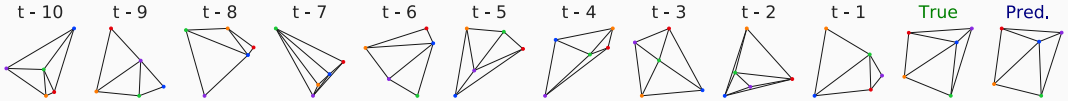
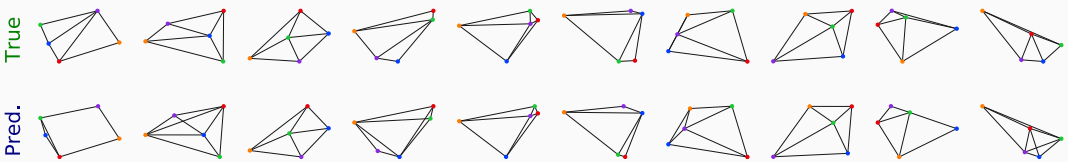
Vector AR

Graphs are represented as vectors $u_t = [\mathrm{vec}(\mathcal{V}_t)^\top, \mathrm{vec}(\mathcal{E}_t)^\top]^\top \in \mathbb{R}^{N \cdot F + N^2}$, and then a linear autoregressive model is applied:

$$\hat{u}_{t+1} = B_0 + \sum_{i=1}^{k} B_i \cdot u_{t-i+1}.$$

Results





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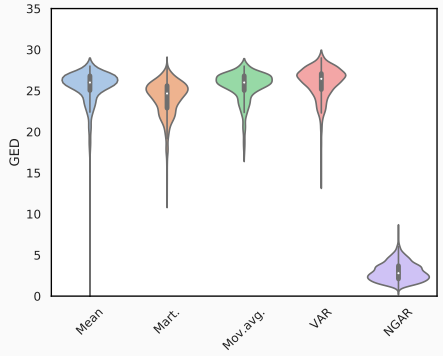


Figure 1: Graph edit distance between predicted and true graphs.

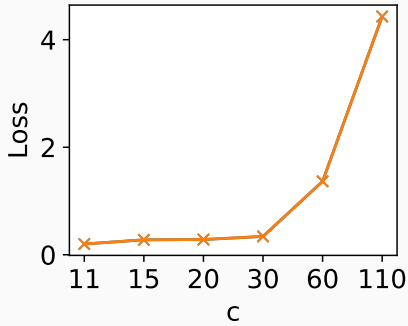


Figure 2: Loss v. complexity of the problem.

Spektral

A library for **relational representation learning**:

- Keras API, TensorFlow backend;
- Includes state-of-the-art GNN layers [2]–[6];
- `danielegrattarola.github.io/spektral`.

Conclusions

Key ideas:

1. Formalized AR models for graphs;
2. GNNs as AR functions from $\mathcal{G}^p$ to $\mathcal{G}$;

Future works:

- Skip graph embedding, work directly in $\mathcal{G}$;
- Improve definition of H.

Code: `https://github.com/dan-zam/NGAR`

D. Grattarola - `grattd@usi.ch` - Twitter: `@riceasphait`

D. Zambon - `zambod@usi.ch`

References i

[1] E. Ott, *Chaos in Dynamical Systems*. Cambridge University Press, 2002.

[2] P. Veličković, G. Cucurull, A. Casanova, A. Romero, P. Liò, and Y. Bengio, "Graph attention networks," *arXiv preprint arXiv:1710.10903*, 2017.

[3] F. M. Bianchi, D. Grattarola, C. Alippi, and L. Livi, "Graph neural networks with convolutional arma filters," *arXiv preprint arXiv:1901.01343*, 2019.

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

[5] 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.

References ii

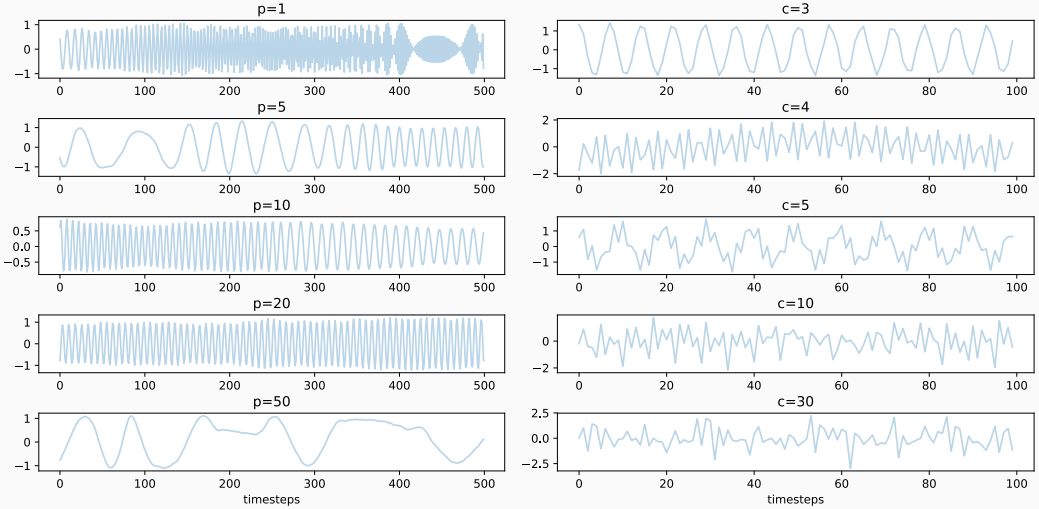
[6] M. Simonovsky and N. Komodakis, "Dynamic edge-conditioned filters in convolutional neural networks on graphs," in *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, 2017.

[7] D. I. Shuman, M. J. Faraji, and P. Vandergheynst, "A multiscale pyramid transform for graph signals," *IEEE Transactions on Signal Processing*, vol. 64, no. 8, pp. 2119–2134, 2016.

[8] 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.

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

Notes on complexity

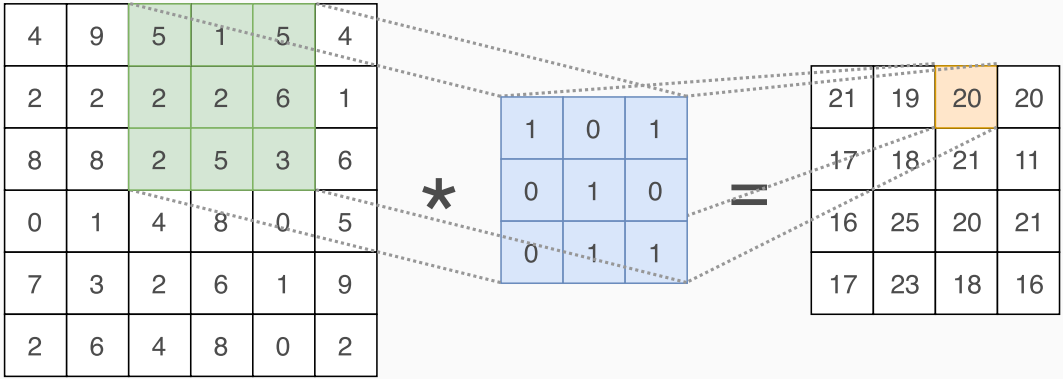


GNNs in one slide

- Graph network blocks: $\mathcal{G} \to \mathcal{G}$.
- Graph pooling blocks: $\mathcal{G}_N \to \mathcal{G}_{M<N}$.
- Differentiable: can be integrated in any deep learning model.
- State of the art in graph representation learning.

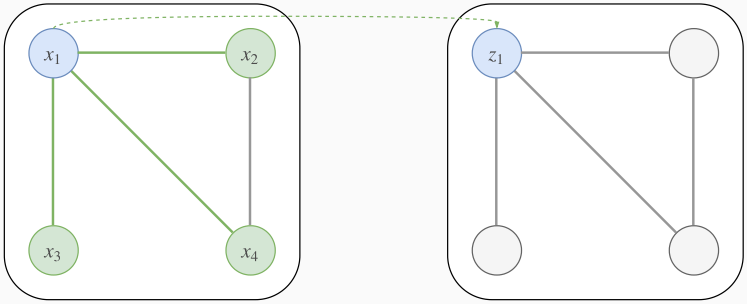
Standard convolution

Convolutional neural networks exploit the spatial locality of pixels.



Graph convolution

Generalise convolutional layers to arbitrary neighbours.



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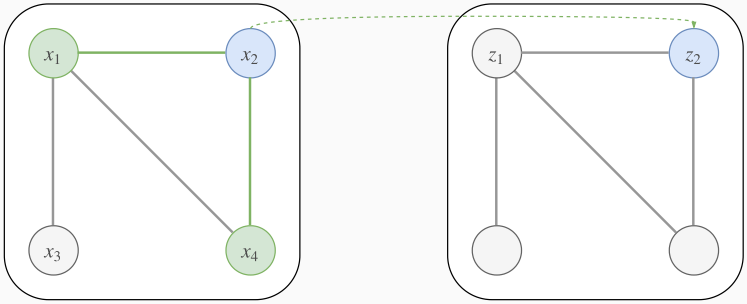

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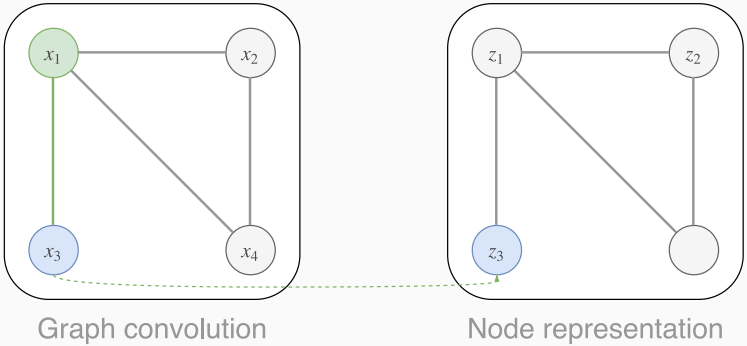

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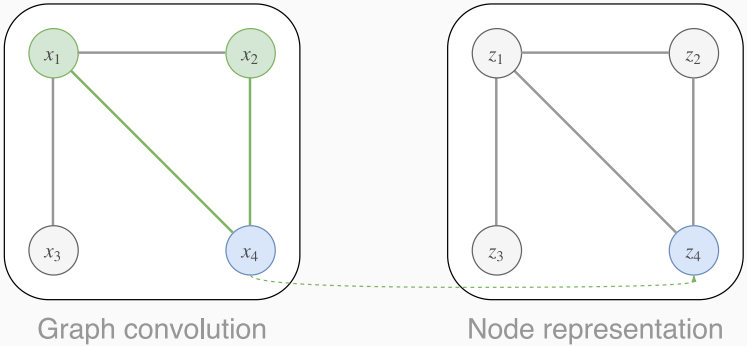

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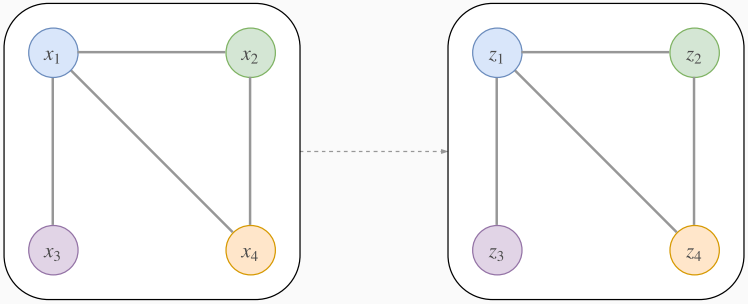

Graph convolution

The output for each node is given by [4]:

$$Z_i = \sum_{j \in \mathcal{N}_i} \tilde{A}_{ij} X_j W + b$$

Can also be written in matrix form:

$$Z = \tilde{A} \cdot X \cdot W + b$$

Note

$\tilde{A}$ can be computed from the adjacency matrix in several ways (e.g., normalised Laplacian [4], row average [6], attention [2], ...)

[2] P. Veličković *et al.*, "Graph Attention Networks," 2017.

[4] T. N. Kipf *et al.*, "Semi-supervised classification with graph convolutional networks," 2016.

[6] M. Simonovsky *et al.*, "Dynamic edge-conditioned filters in convolutional neural networks on graphs," 2017.

Graph convolution

We can take edge features into account by replacing W with a neural network that transforms edge features into convolutional kernels [6]:

$$Z_i = \sum_{j \in \mathcal{N}(i)} \tilde{A}_{ij} \cdot X_j \cdot W + b$$

becomes

$$Z_i = \sum_{j \in \mathcal{N}(i)} \tilde{A}_{ij} \cdot X_j \cdot f(E_{ji}) + b$$

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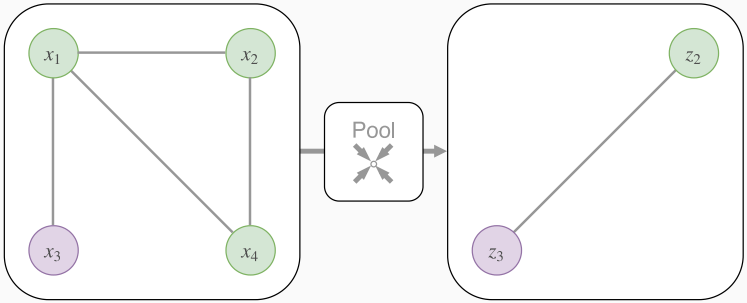
Graph pooling

Aggregate node features to obtain a lower-resolution graph [5], [7], [8].



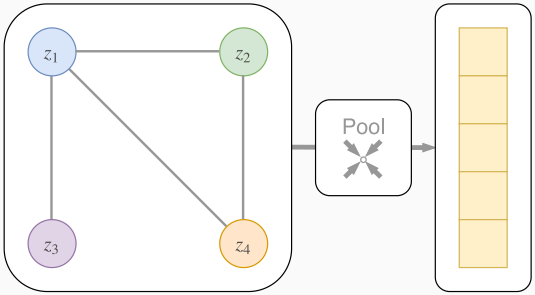
[5] M. Defferrard *et al.*, "Convolutional neural networks on graphs with fast localized spectral filtering," 2016.

[7] D. I. Shuman *et al.*, "A multiscale pyramid transform for graph signals," 2016.

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

Graph pooling

Global pooling is the final step to reduce a graph to a vector, e.g., $Z = \sum_i \alpha_i X_i$.



α_i can be learned with neural network $f(X) : \mathbb{R}^{N \times F} \to [0, 1]^N$ to compute the relative importance of each node [9].

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