MotifNet: a Motif-based GCNN for Directed Graphs

Federico Monti[1,2], Karl Otness[5], Michael M. Bronstein[1,2,3,4,5]

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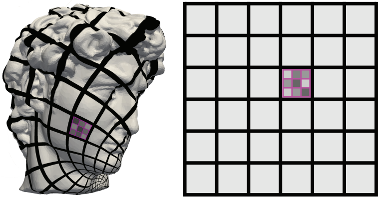
Different formulations of CNN on graphs

Spectral domain[1,2,3]

Spatial domain[4,5,6]



Embedding domain[7,8]

[1]Bruna et al. 2014; [2]Henaff, Bruna, LeCun 2015; [3]Defferrard, Bresson, Vandergheynst 2016; [4]Masci et al. 2015; [5]Boscaini et al. 2016; [6]Monti et al. 2017; [7]Sinha, Bai, Ramani 2016; [8]Maron et al. 2017

Directed graphs

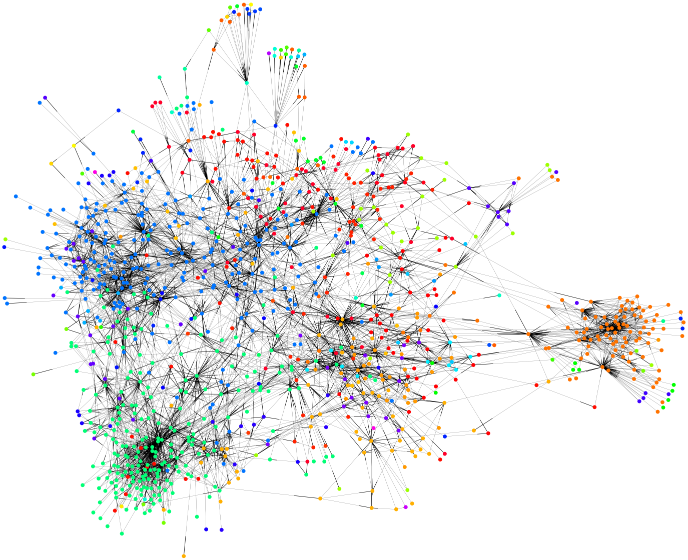


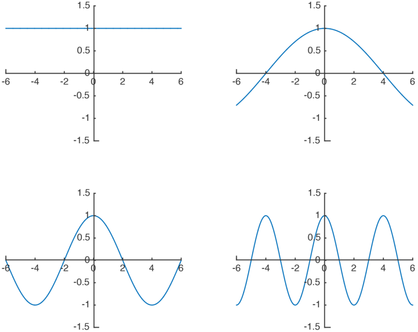
Figure: Monti, Otness, Bronstein 2018; data: Bojchevski, Günnemann 2017

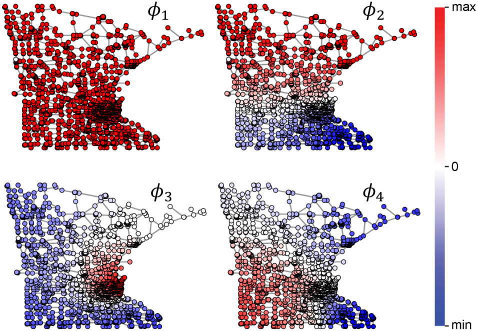
Graph Convolutional Neural Networks

Laplacian eigenfunctions

$$\Delta e^{j\omega x} = \frac{d^2}{dx^2} e^{j\omega x} = -\omega^2 e^{j\omega x}$$

$$\mathbf{\Delta} = \mathbf{D} - \mathbf{W} = \mathbf{\Phi} \mathbf{\Lambda} \mathbf{\Phi}^{\mathrm{T}}$$





Convolution Theorem

- Given two functions $f, h : Z \to \mathbb{R}$ their convolution is a function

$$(f \star h)(x) = \sum_{x'=-K/2}^{K/2} f(x - x')h(x') = \mathcal{F}^{-1}\{\mathcal{F}\{f\} \cdot \mathcal{F}\{h\}\}$$

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- Given two functions $f, h : \mathcal{V} \to \mathbb{R}$ their convolution is a function

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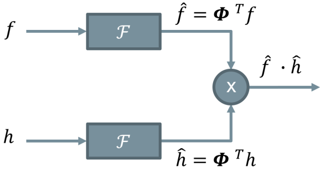

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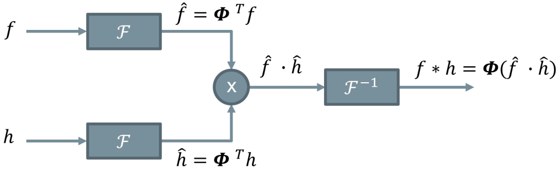

$$f * h = \boldsymbol{\Phi}\,(\boldsymbol{\Phi}^T h) \cdot (\boldsymbol{\Phi}^T f)$$

Spectral graph CNN

Convolutional layer expressed in the spectral domain

$$\mathbf{g}_l = \xi \left(\sum_{l'=1}^{p} \mathbf{\Phi} \begin{bmatrix} \hat{h}_1^{(l,l')} & & \\ & \ddots & \\ & & \hat{h}_N^{(l,l')} \end{bmatrix} \mathbf{\Phi}^\top \mathbf{f}_{l'} \right) \qquad \begin{array}{l} l = 1, \ldots, q \\ l' = 1, \ldots, p \end{array}$$

where q is the number of features in output and p in input.

Bruna et al. 2014

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where q is the number of features in output and p in input.

- ☹ $\mathcal{O}(N)$ parameters per layer
- ☹ $\mathcal{O}(N^2)$ computation of forward and inverse Fourier transforms $\mathbf{\Phi}^\top, \mathbf{\Phi}$ (no FFT on graphs)
- ☹ No guarantee of spatial localization of filters

Bruna et al. 2014

Spectral graph CNN with polynomial filters

Represent spectral transfer function as a polynomial or order r

$$\tau_{\boldsymbol{\alpha}}(\lambda) = \sum_{j=0}^{r} \alpha_j \lambda^j$$

where $\boldsymbol{\alpha} = (\alpha_0, \ldots, \alpha_r)^\top$ is the vector of filter parameters

Defferrard, Bresson, Vandergheynst 2016

Spectral graph CNN with polynomial filters

Represent spectral transfer function as a Chebyshev polynomial or order r

$$\tau_{\boldsymbol{\alpha}}(\tilde{\lambda}) = \sum_{j=0}^{r} \alpha_j T_j(\tilde{\lambda})$$

where $\boldsymbol{\alpha} = (\alpha_0, \ldots, \alpha_r)^\top$ is the vector of filter parameters,

$$T_j(\tilde{\lambda}) = 2\tilde{\lambda}T_{j-1}(\tilde{\lambda}) - T_{j-2}(\tilde{\lambda}) \qquad T_0(\tilde{\lambda}) = 1, \quad T_1(\tilde{\lambda}) = \tilde{\lambda}$$

and $-1 \leq \tilde{\lambda} \leq 1$ is normalized frequency.

Defferrard, Bresson, Vandergheynst 2016

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and $-1 \leq \tilde{\lambda} \leq 1$ is normalized frequency.

Application of the filter to scaled Laplacian $\tilde{\boldsymbol{\Delta}} = \mathbf{D}^{-0.5} \boldsymbol{\Delta} \mathbf{D}^{-0.5} - \mathbf{I} = \boldsymbol{\Phi} \tilde{\boldsymbol{\Lambda}} \boldsymbol{\Phi}^T$:

$$\mathbf{g} = \boldsymbol{\Phi}(\sum_{j=0}^{r} \alpha_j T_j(\tilde{\boldsymbol{\Lambda}}))\boldsymbol{\Phi}^T \mathbf{f} = \sum_{j=0}^{r} \alpha_j T_j(\tilde{\boldsymbol{\Delta}})\mathbf{f}$$

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- ☺ $\mathcal{O}(1)$ parameters per layer
- ☺ Filters have guaranteed r-hops support
- ☺ No explicit computation of $\boldsymbol{\Phi}^\top, \boldsymbol{\Phi} \Rightarrow \mathcal{O}(r|\mathcal{E}|)$ computational complexity

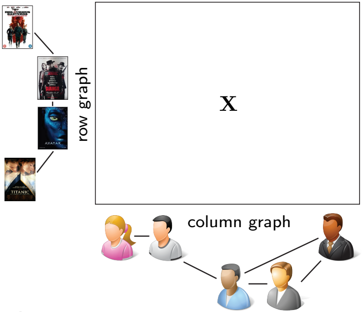
Defferrard, Bresson, Vandergheynst 2016

Multi-Graph CNN

Multi-graph spectral convolutional layer

$$\mathbf{Y}_l = \xi\left(\sum_{l'=1}^{p}\sum_{j,j'=0}^{r}\theta_{jj'll'}T_j(\tilde{\boldsymbol{\Delta}}_{\mathrm{r}})\mathbf{X}_{l'}T_{j'}(\tilde{\boldsymbol{\Delta}}_{\mathrm{c}})\right) \quad \begin{matrix} l = 1,\ldots,q \\ l' = 1,\ldots,p \end{matrix}$$

applied to p input channels ($m \times n$ matrices $\mathbf{X}_1,\ldots,\mathbf{X}_p$) and producing q output channels ($m \times n$ matrices $\mathbf{Y}_1,\ldots,\mathbf{Y}_q$)



Monti, Bresson, Bronstein 2017

Multi-Graph CNN

Multi-graph spectral convolutional layer

$$\mathbf{Y}_l = \xi\left(\sum_{l'=1}^{p}\sum_{j,j'=0}^{r}\theta_{jj'll'}T_j(\tilde{\boldsymbol{\Delta}}_{\mathrm{r}})\mathbf{X}_{l'}T_{j'}(\tilde{\boldsymbol{\Delta}}_{\mathrm{c}})\right) \quad \begin{array}{l} l = 1,\ldots,q \\ l' = 1,\ldots,p \end{array}$$

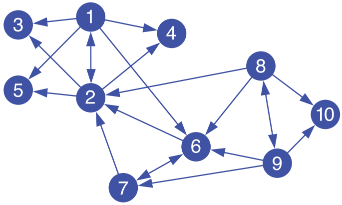
applied to p input channels ($m \times n$ matrices $\mathbf{X}_1,\ldots,\mathbf{X}_p$) and producing q output channels ($m \times n$ matrices $\mathbf{Y}_1,\ldots,\mathbf{Y}_q$)

- ☺ $\mathcal{O}(1)$ parameters per layer
- ☺ Filters have guaranteed r-hops support on both graphs
- ☺ $\mathcal{O}(nm)$ computational complexity

Monti, Bresson, Bronstein 2017

Dealing with Directed Graphs

Directed graphs

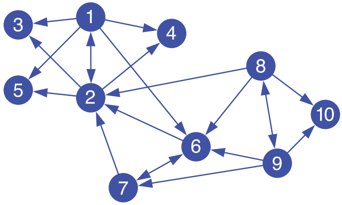


Directed graph

Asymmetric adjacency matrix

$$\begin{bmatrix}
. & 1 & 1 & 1 & 1 & 1 & . & . & . & . \\
1 & . & 1 & 1 & 1 & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . \\
. & 1 & . & . & . & . & 1 & . & . & . \\
. & 1 & . & . & . & 1 & . & . & . & . \\
. & 1 & . & . & . & 1 & . & . & 1 & 1 \\
. & . & . & . & . & 1 & 1 & 1 & . & 1 \\
. & . & . & . & . & . & . & . & . & .
\end{bmatrix}$$

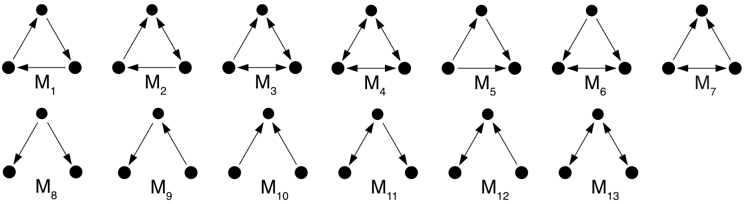
Motif-based graph analysis



Directed graph

Asymmetric adjacency matrix

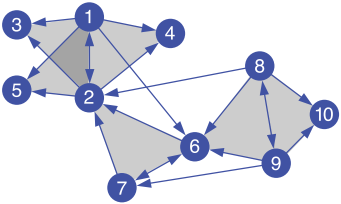
$$\begin{bmatrix} . & 1 & 1 & 1 & 1 & 1 & . & . & . & . \\ 1 & . & 1 & 1 & 1 & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . \\ . & 1 & . & . & . & . & 1 & . & . & . \\ . & 1 & . & . & . & 1 & . & . & . & . \\ . & 1 & . & . & . & 1 & . & . & 1 & 1 \\ . & . & . & . & . & 1 & 1 & 1 & . & 1 \\ . & . & . & . & . & . & . & . & . & . \end{bmatrix}$$



Graph motifs

Benson et al. 2016

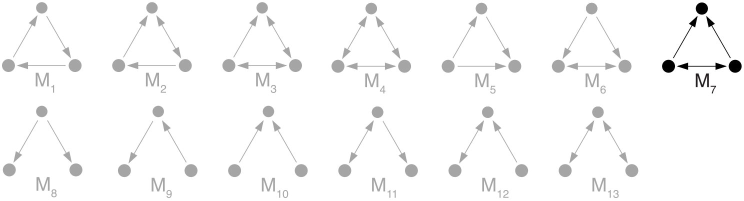
Motif-based graph analysis



Directed graph

Motif adjacency matrix for M_7

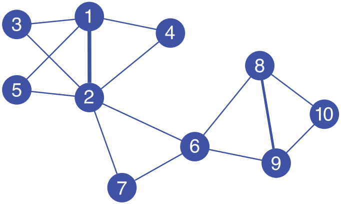
$$\begin{bmatrix}
. & 3 & 1 & 1 & 1 & . & . & . & . & . \\
3 & . & 1 & 1 & 1 & 1 & 1 & . & . & . \\
1 & 1 & . & . & . & . & . & . & . & . \\
1 & 1 & . & . & . & . & . & . & . & . \\
1 & 1 & . & . & . & . & . & . & . & . \\
. & 1 & . & . & . & . & 1 & 1 & 1 & . \\
. & 1 & . & . & . & 1 & . & . & . & . \\
. & . & . & . & . & 1 & . & . & 2 & 1 \\
. & . & . & . & . & 1 & . & 2 & . & 1 \\
. & . & . & . & . & . & . & 1 & 1 & .
\end{bmatrix}$$



Graph motifs

Benson et al. 2016

Motif Laplacians



Undirected weighted graph

Motif adjacency matrix for M_7

$$\begin{bmatrix} . & 3 & 1 & 1 & 1 & . & . & . & . & . \\ 3 & . & 1 & 1 & 1 & 1 & 1 & . & . & . \\ 1 & 1 & . & . & . & . & . & . & . & . \\ 1 & 1 & . & . & . & . & . & . & . & . \\ 1 & 1 & . & . & . & . & . & . & . & . \\ . & 1 & . & . & . & . & 1 & 1 & 1 & . \\ . & 1 & . & . & . & 1 & . & . & . & . \\ . & . & . & . & . & 1 & . & . & 2 & 1 \\ . & . & . & . & . & 1 & . & 2 & . & 1 \\ . & . & . & . & . & . & . & 1 & 1 & . \end{bmatrix}$$

Motif Laplacian for motif $k = 1, \ldots, K$

$$\tilde{\mathbf{\Delta}}_k = \mathbf{I} - \tilde{\mathbf{D}}_k^{-1/2} \tilde{\mathbf{W}}_k \tilde{\mathbf{D}}_k^{-1/2}$$

Benson et al. 2016

MotifNet: multivariate polynomial

Apply K-variate polynomial of order r to the motif Laplacians

$$\tau_{\boldsymbol{\theta}}(\tilde{\boldsymbol{\Delta}}_1, \ldots, \tilde{\boldsymbol{\Delta}}_K) = \theta_0 \mathbf{I} + \sum_{j=1}^{r} \sum_{k_1, \ldots, k_j \in \{1, \ldots, K\}} \theta_{k_1, \ldots, k_j} \tilde{\boldsymbol{\Delta}}_{k_1} \cdots \tilde{\boldsymbol{\Delta}}_{k_j}$$

where $\boldsymbol{\theta} = (\theta_0, \theta_1, \ldots, \theta_{K, \ldots, K})$ is the vector of filter parameters

Monti, Otness, Bronstein 2018

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☺ Explicitly accounts for directed graph structures

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☺ Anisotropic kernels

Monti, Otness, Bronstein 2018

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- ☺ Anisotropic kernels
- ☺ Filters have guaranteed r-hops support

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- ☺ Explicitly accounts for directed graph structures
- ☺ Anisotropic kernels
- ☺ Filters have guaranteed r-hops support
- ☺ $\mathcal{O}(1)$ parameters per layer

Monti, Otness, Bronstein 2018

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- ☺ Anisotropic kernels
- ☺ Filters have guaranteed r-hops support
- ☹ $\frac{1-K^{r+1}}{1-K}$ parameters per layer, intractable in practice

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- ☹ $\frac{1-K^{r+1}}{1-K}$ parameters per layer, intractable in practice
- ☹ $\mathcal{O}(n\frac{1-K^{r+1}}{1-K})$ computational complexity

Monti, Otness, Bronstein 2018

MotifNet: simplified multivariate polynomial

Two possible simplications:

- We consider only $K = 2$ simple motifs corresponding to incoming and outgoing edges (MotifNet-d):

$$\tau_{\boldsymbol{\theta}} = \theta_0 \mathbf{I} + \theta_1 \tilde{\boldsymbol{\Delta}}_1 + \theta_2 \tilde{\boldsymbol{\Delta}}_2 + \theta_{11} \tilde{\boldsymbol{\Delta}}_1^2 + \ldots + \theta_{22} \tilde{\boldsymbol{\Delta}}_2^2 + \ldots \tag{1}$$

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- We consider a simplified version of multivariate polynomials (MotifNet-m) defined recursively as:

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- We consider a simplified version of multivariate polynomials (MotifNet-m) defined recursively as:

$$\begin{aligned}
\mathbf{P}_{\boldsymbol{\Theta}}(\tilde{\boldsymbol{\Delta}}_1, \ldots, \tilde{\boldsymbol{\Delta}}_K) &= \sum_{j=0}^{r} \theta_j \mathbf{P}_j; \qquad (2) \\
\mathbf{P}_j(\tilde{\boldsymbol{\Delta}}_1, \ldots, \tilde{\boldsymbol{\Delta}}_K) &= \sum_{k=1}^{K} \alpha_{k,j} \tilde{\boldsymbol{\Delta}}_k \mathbf{P}_{j-1}, \quad j = 1, \ldots, p \\
\mathbf{P}_0 &= \mathbf{I}, \\
\sum_{k=1}^{K} \alpha_{k,j} &= 1 \qquad j = 1, \ldots, p
\end{aligned}$$

Monti, Otness, Bronstein 2018

MotifNet-m: simplified multivariate polynomial

Apply attention-based recursive polynomial of order r

$$\mathbf{P}_{\boldsymbol{\Theta}}(\tilde{\boldsymbol{\Delta}}_1, \ldots, \tilde{\boldsymbol{\Delta}}_K) = \sum_{j=0}^{r} \theta_j \mathbf{P}_j;$$

$$\mathbf{P}_j(\tilde{\boldsymbol{\Delta}}_1, \ldots, \tilde{\boldsymbol{\Delta}}_K) = \sum_{k=1}^{K} \alpha_{k,j} \tilde{\boldsymbol{\Delta}}_k \mathbf{P}_{j-1}, \qquad \mathbf{P}_0 = \mathbf{I},$$

where $\boldsymbol{\Theta} = (\theta_0, \ldots, \theta_r, \alpha_{1,1}, \ldots, \alpha_{K,r})$ is the vector of filter parameters

- ☺ Explicitly accounts for directed graph structures
- ☺ Anisotropic kernels
- ☺ Filters have guaranteed r-hops support

Monti, Otness, Bronstein 2018

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- ☺ Explicitly accounts for directed graph structures
- ☺ Anisotropic kernels
- ☺ Filters have guaranteed r-hops support
- ☺ $Kr + 1$ parameters per layer

Monti, Otness, Bronstein 2018

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- ☺ Anisotropic kernels
- ☺ Filters have guaranteed r-hops support
- ☺ $Kr + 1$ parameters per layer
- ☺ $\mathcal{O}(nr)$ computational complexity

Monti, Otness, Bronstein 2018

Directed CORA

- Citations network representing papers (vertices) and citations (directed edges)
- Goal: vertex-wise classification (paper topic)
- 19,793 documents, 70 classes
- Training/validation/test set: 10% samples (1979 vertices)

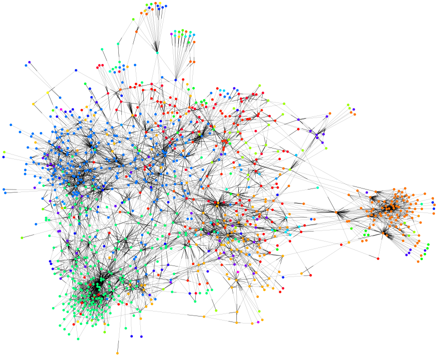
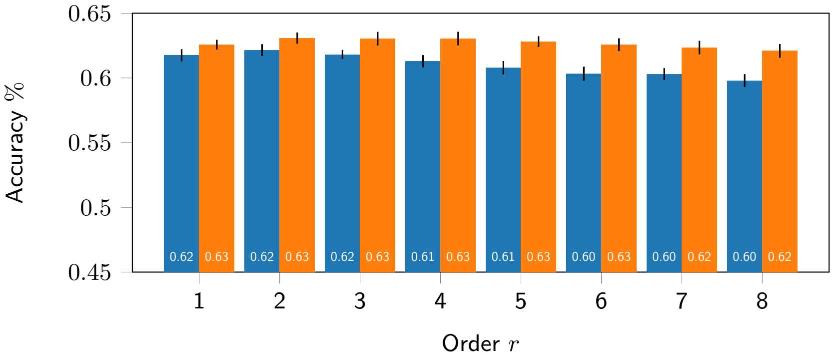


Figure: Monti, Otness, Bronstein 2018; data: Bojchevski, Günnemann 2017

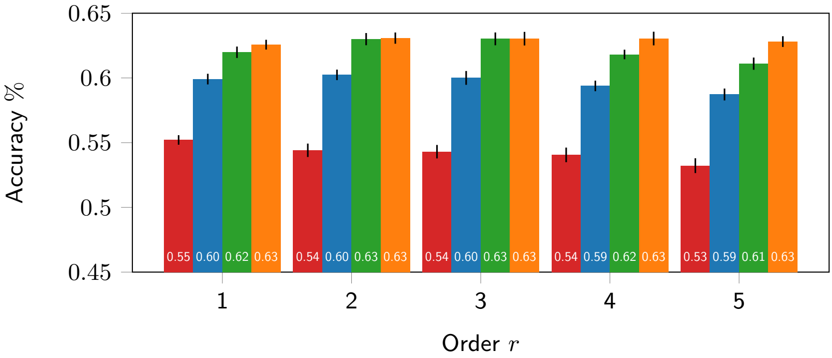
Example: directed citation networks (CORA)



Classification accuracy obtained with ChebNet on undirected graph (blue) and MotifNet-m (orange).

Monti, Otness, Bronstein 2018; data: Bojchevski, Günnemann, 2017

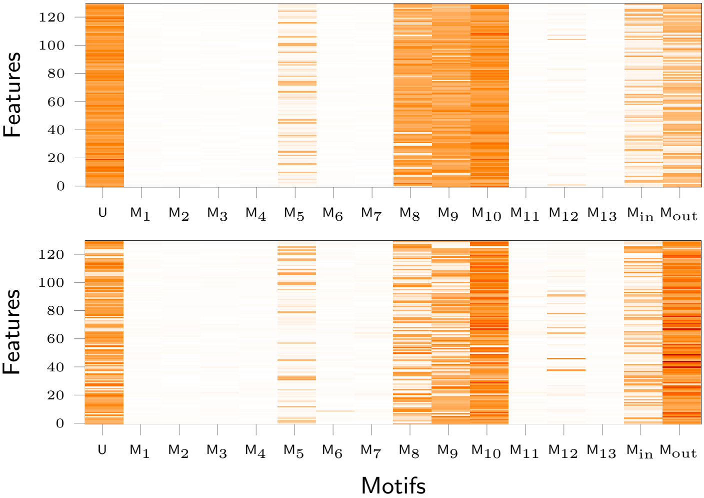
Example: directed citation networks (CORA)



Classification accuracy obtained with ChebNet applied with directed adjacency matrix $\mathbf{W}$ (blue) / $\mathbf{W}^\top$ (red), MotifNet-d (green) and MotifNet-m (orange).

Monti, Otness, Bronstein 2018; data: Bojchevski, Günnemann, 2017

Example: directed citation networks (CORA)



Attention scores α obtained with MotifNet-m ($r = 1$) from 1st and 2nd graph convolutional layers. Dark/bright colors represent high/low probabilities.

Monti, Otness, Bronstein 2018; data: Bojchevski, Günnemann, 2017

Conclusions

- We presented MotifNet, a motif-based GCN for directed graphs.
- Our solution realizes anisotropic filters on the provided domain generalizing and enriching classic undirected GCNs.
- Thanks to the proposed simplifications, MotifNet-m requires a number of parameters and a computational complexity comparable with the ones of ChebNet.
- Experimental evaluations on the directed version of CORA show the superior performance of our approach.

Thank You

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