Data Science Training

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Deep Learning on Graphs

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Outline

- **Convolutional Neural Networks**
  - *Architecture*
  - *Non-Euclidean Data*
- **Spectral Graph Theory**
  - *Graphs and operators*
  - *Spectral decomposition*
  - *Fourier analysis*
  - *Convolution*
  - *Coarsening*
- **Spectral ConvNets**
  - *SplineNets*
  - *ChebNets*
  - *GraphConvNets*
- **Spectral ConvNets on Multiple Graphs**
  - *Recommender Systems*
- **Conclusion**

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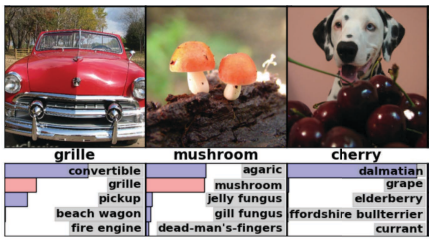
Convolutional neural networks[1]

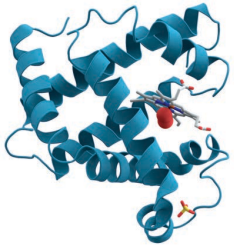
- Data (image, video, sound) are compositional, i.e. they are formed of patterns that are:
  - Local
  - Stationary
  - Multi-scale (/hierarchical)

- ConvNets leverage the compositionality structure: They extract compositional features and feed them to classifier, recommender, etc (end-to-end).

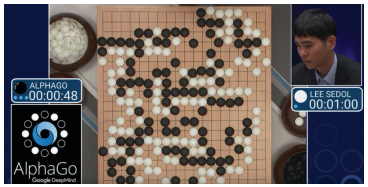


Computer Vision

NLP



Drug discovery

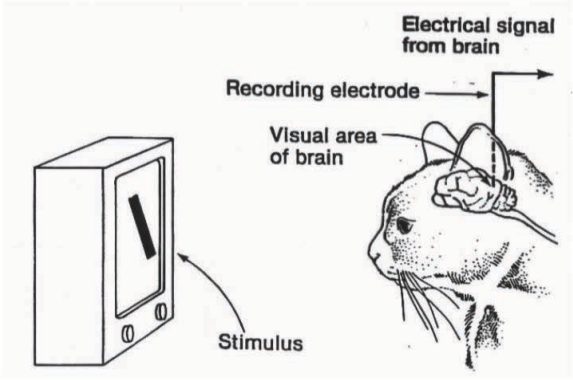


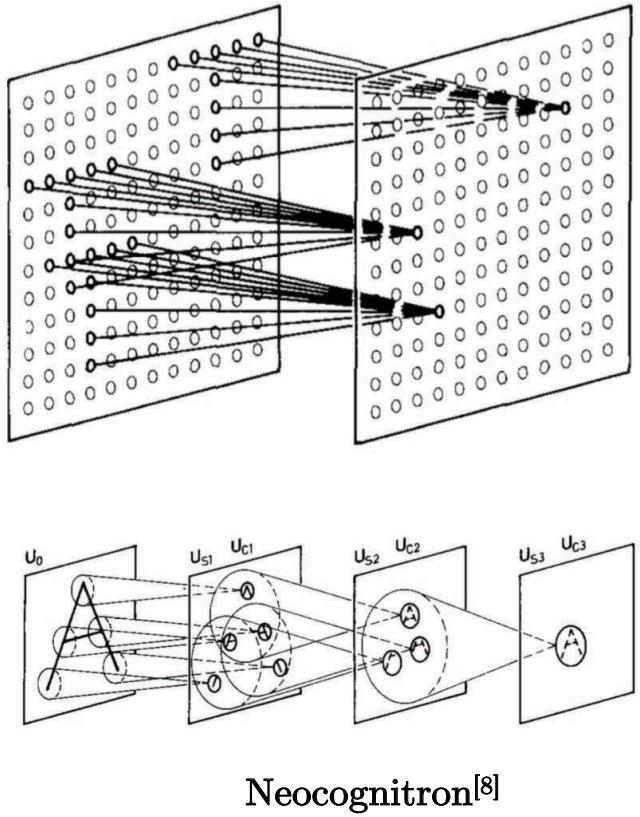
Games

[1] LeCun et al. 1998

Key properties

- Locality: Property inspired by visual cortex neurons[7].
- Local receptive fields activate in the presence of (learned) local features.



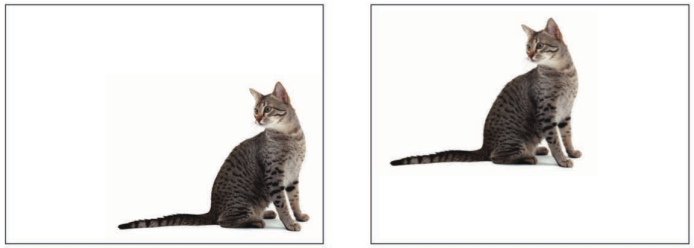


Neocognitron[8]

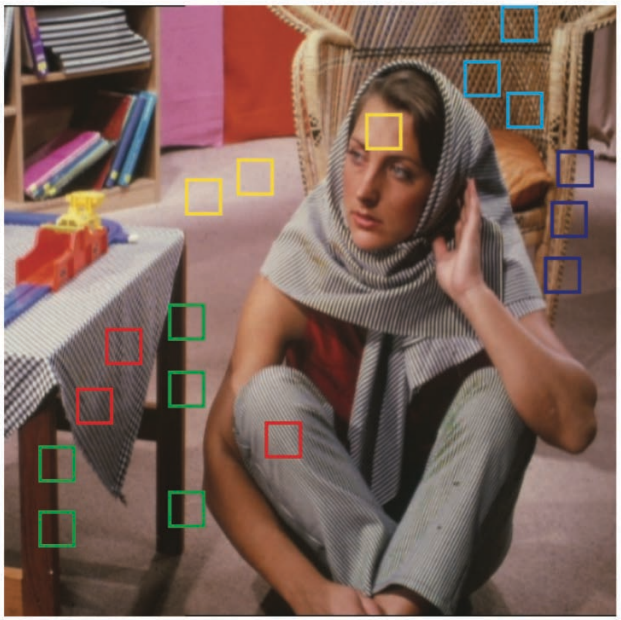
[7] Cybenko 1989, Hornik 1991, [8] Fukushima 1980

Key properties

- Stationarity $\Leftrightarrow$ Translation invariance

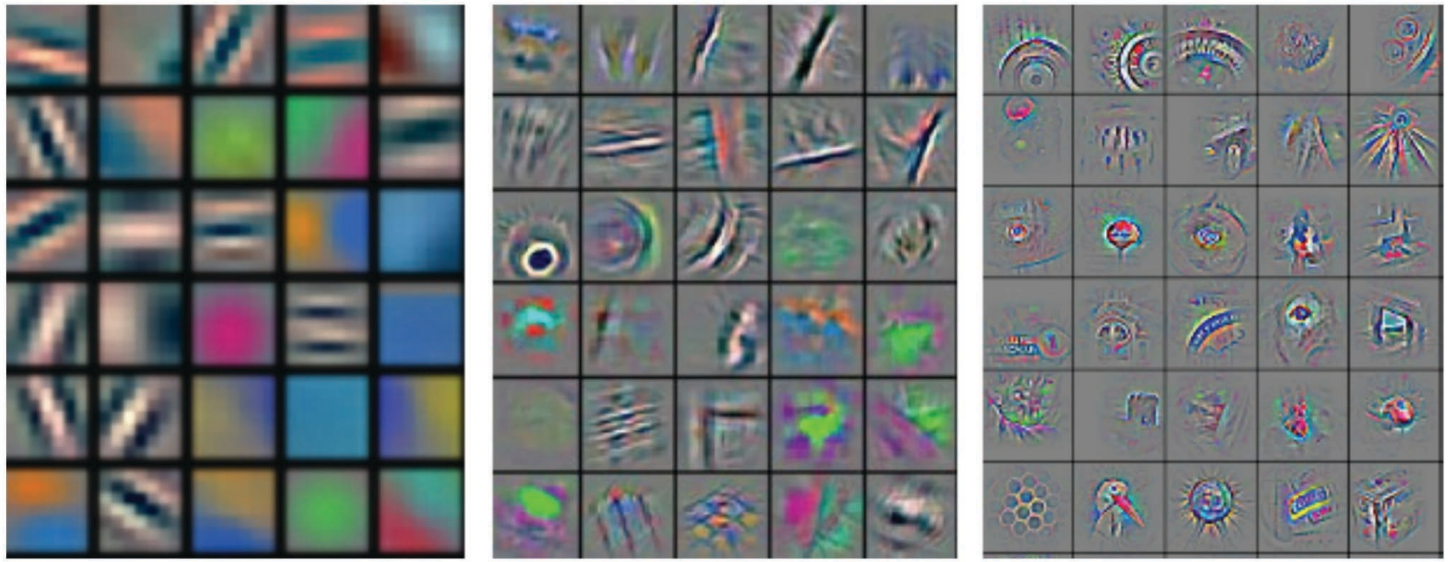


- Local stationarity $\Leftrightarrow$ Similar patches shared across the data domain.



Key properties

- Multi-scale: Simple structures combine to compose slightly more abstract structures, and so on, in a hierarchical way.
- Also inspired by brain visual primary cortex (V1 and V2 neurons).

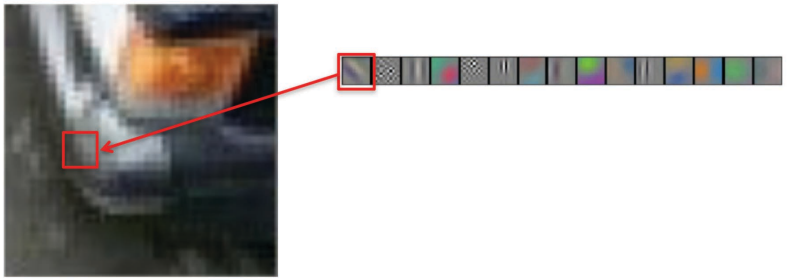


Features learned by a ConvNet become increasingly complex at deeper layers.[9]

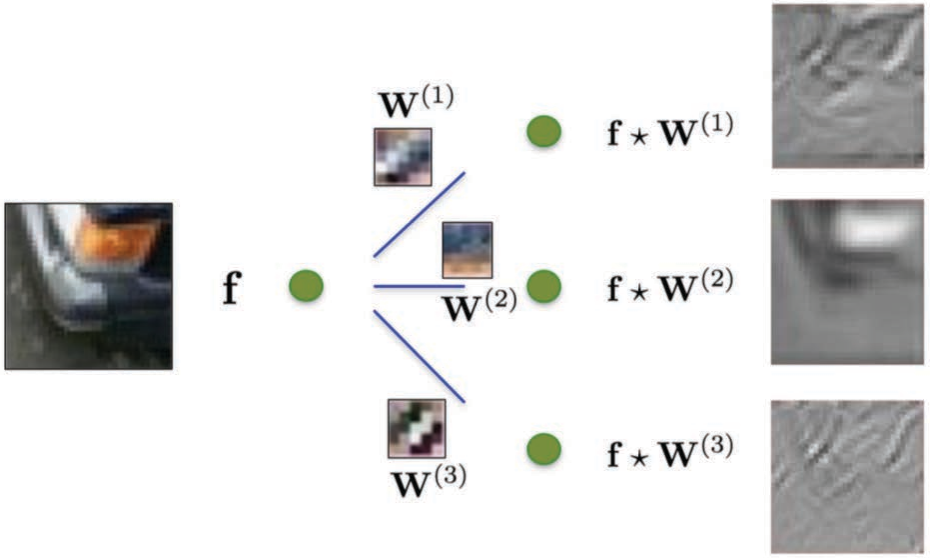
[9] Zeiler, Fergus 2013

Implementation

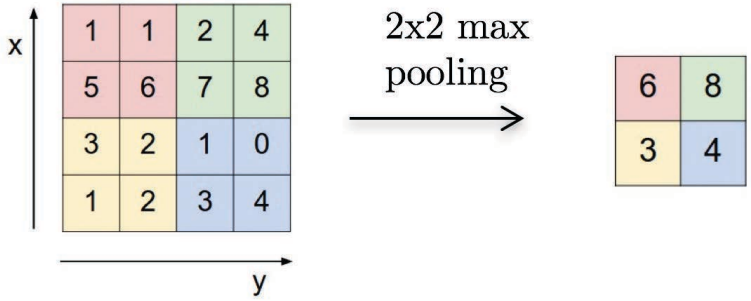
- Locality: compact support kernels $\Rightarrow$ O(1) parameters per filter.



- Stationarity: convolutional operators $\Rightarrow$ O($n$log$n$) in general (FFT) and O(n) for compact kernels.

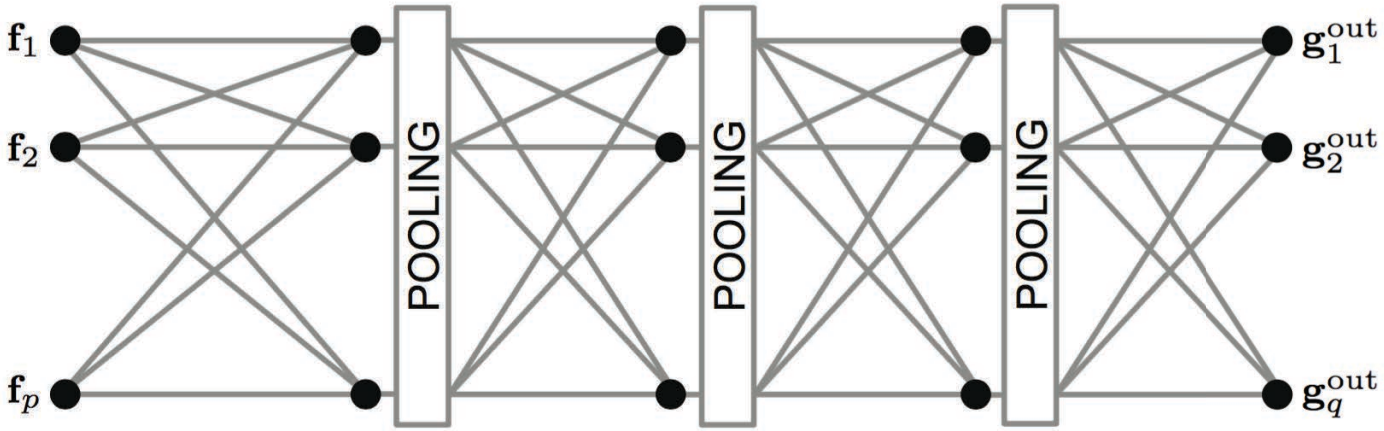


- Multi-scale: downsampling + pooling $\Rightarrow$ O(n)



Compositional features

$$\begin{aligned} \mathbf{f}_l &= l\text{-th image feature (R,G,B channels), } \dim(\mathbf{f}_l) = n \times 1 \\ \mathbf{g}_l^{(k)} &= l\text{-th feature map, } \dim(\mathbf{g}_l^{(k)}) = n_l^{(k)} \times 1 \end{aligned}$$



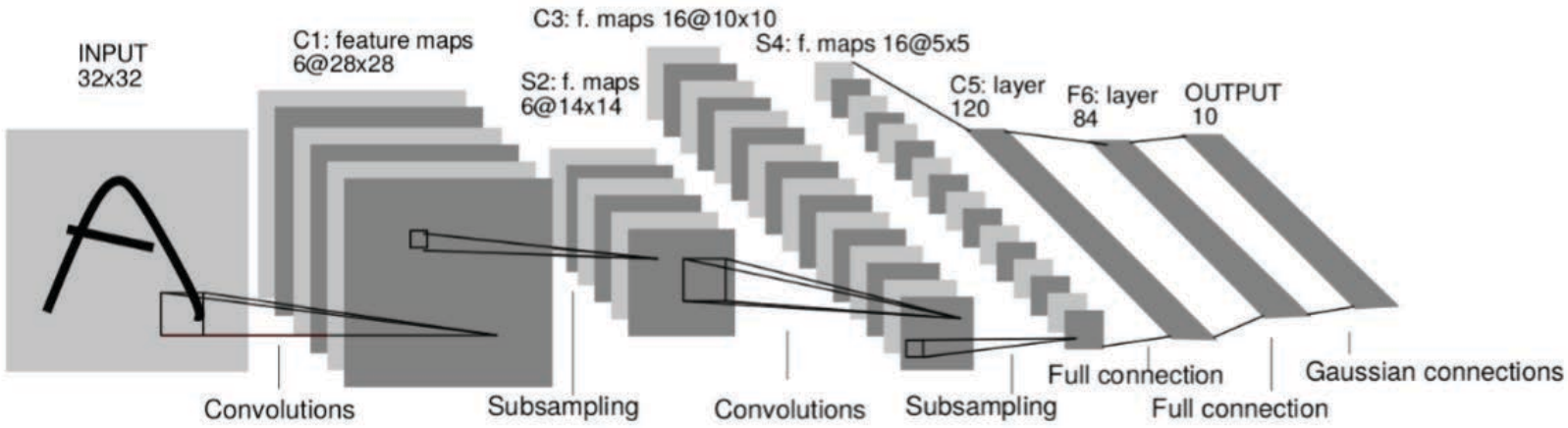
Compositional features consist of multiple convolutional + pooling layers.

Linear layer $$\mathbf{g}_l^{(k)} = \xi\left(\sum_{l'=1}^{q_{k-1}} \mathbf{W}_{l,l'}^{(k)} \star \xi\left(\sum_{l'=1}^{q_{k-2}} \mathbf{W}_{l,l'}^{(k-1)} \star \xi\left(\cdots \mathbf{f}_{l'}\right)\right)\right)$$

Activation, e.g. $\xi(x) = \max\{x, 0\}$ rectified linear unit (ReLU)

Pooling $$\mathbf{g}_l^{(k)}(x) = \|\mathbf{g}_l^{(k-1)}(x') : x' \in \mathcal{N}(x)\|_p \quad p = 1, 2, \text{ or } \infty$$

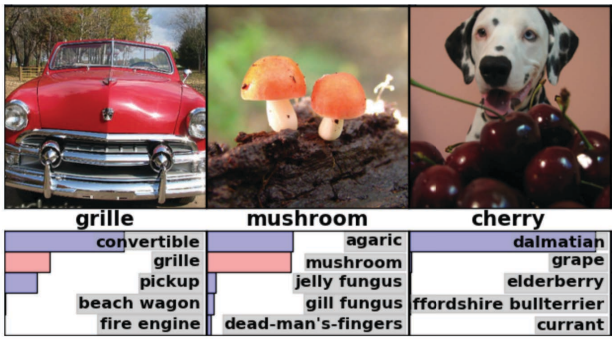
ConvNets[1]



- ☺ Filters localized in space (Locality)
- ☺ Convolutional filters (Stationarity)
- ☺ Multiple layers (Multi-scale)
- ☺ O(1) parameters per filter (independent of input image size n)
- ☺ O(n) complexity per layer (filtering done in the spatial domain)

[1] LeCun et al. 1998

ConvNets in computer vision



Image/object recognition

[Krizhevsky-Sutskever-Hinton'12]

Image inpainting

[Pathak-Efros-etal'16]

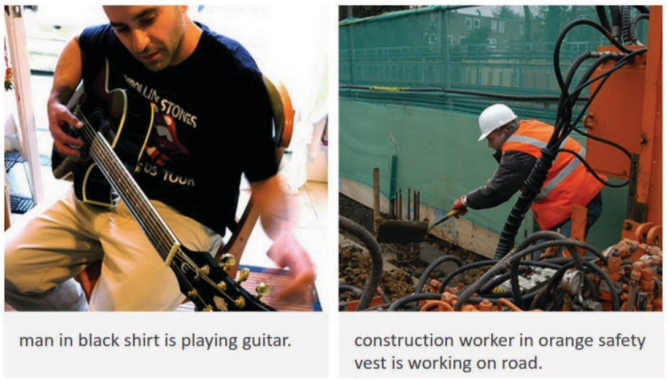


Image captioning

[Karpathy-Li'15]

Self-driving cars

⇒ Highly successful - ConvNets is the Swiss knife of Computer Vision!

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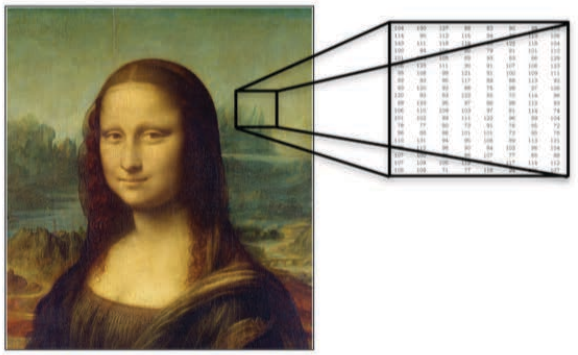
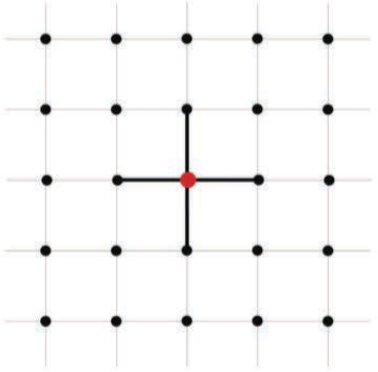
Data domain for ConvNets

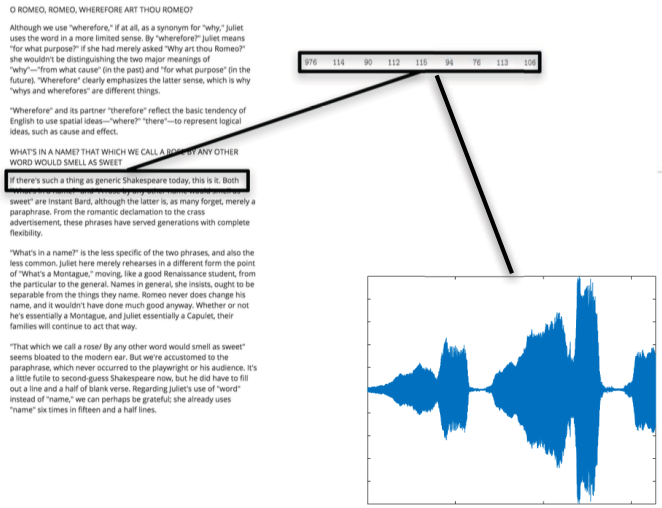
- Image, volume, video: 2D, 3D, 2D+1 Euclidean domains





2D grids

- Sentence, word, sound: 1D Euclidean domain



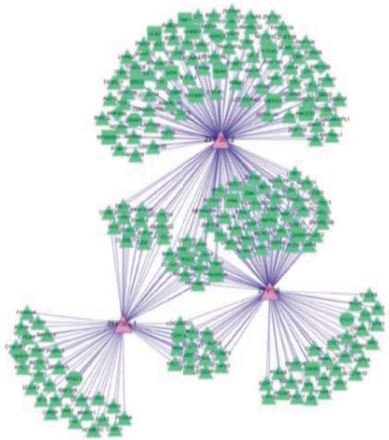
1D grid

- These domains have nice regular spatial structures.

  $\Rightarrow$ All CNN operations are math well defined and fast (convolution, pooling).

Non-Euclidean data

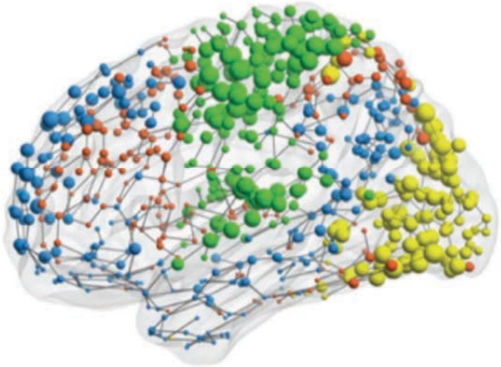
Social networks



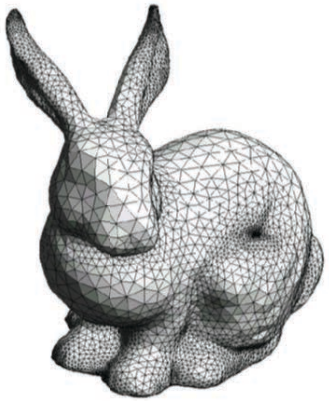
Regulatory networks

=

Graphs/
Networks



Functional networks



3D shapes

- Also NLP, physics, social science, communication networks, etc.

Challenges of graph deep learning

- Extend neural network techniques to graph-structured data.
- Assumption: Non-Euclidean data are locally stationary and manifest hierarchical structures.
- How to define compositionality on graphs? (convolution and pooling on graphs)
- How to make them fast? (linear complexity)

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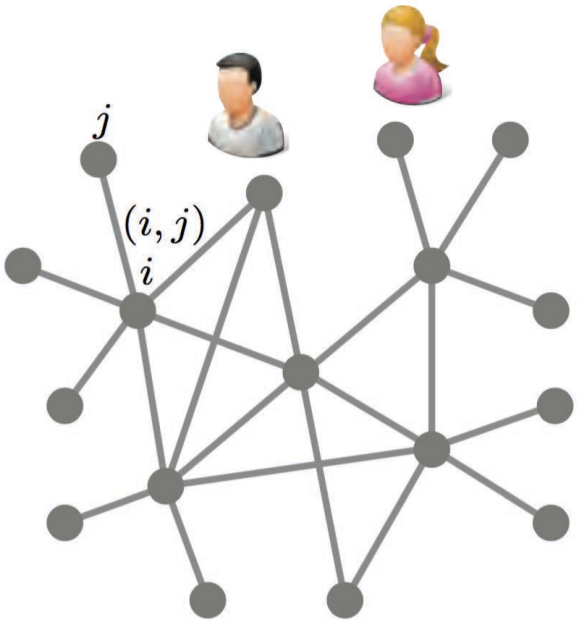
Graphs[10]

- Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$
- Vertices $\mathcal{V} = \{1, \ldots, n\}$
- Edges $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$
- Vertex weights $b_i > 0$ for $i \in \mathcal{V}$
- Edge weights $a_{ij} \geq 0$ for $(i, j) \in \mathcal{E}$
- Vertex fields $L^2(\mathcal{V}) = \{f : \mathcal{V} \to \mathbb{R}^h\}$
  Represented as $\mathbf{f} = (f_1, \ldots, f_n)$
- Hilbert space with inner product

$$\langle f, g \rangle_{L^2(\mathcal{V})} = \sum_{i \in \mathcal{V}} a_i f_i g_i$$



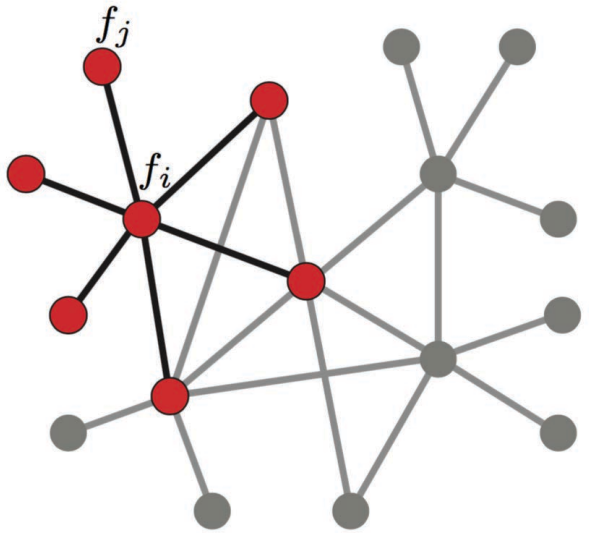
[10] Chung 1994

Graph Laplacian

- Laplacian operator $\Delta : L^2(\mathcal{V}) \to L^2(\mathcal{V})$

$$(\Delta f)_i = \frac{1}{b_i} \sum_{j:(i,j)\in\mathcal{E}} a_{ij}(f_i - f_j)$$

difference between f and its local average (2nd derivative on graphs)



- Core operator in spectral graph theory.
- Represented as a positive semi-definite $n \times n$ matrix
  - Unnormalized Laplacian $\mathbf{\Delta} = \mathbf{D} - \mathbf{A}$
  - Normalized Laplacian $\mathbf{\Delta} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$
  - Random walk Laplacian $\mathbf{\Delta} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{A}$

where $\mathbf{A} = (a_{ij})$ and $\mathbf{D} = \mathrm{diag}(\sum_{j\neq i} a_{ij})$

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Spectral decomposition

- A Laplacian of a graph of n vertices admits n eigenvectors

$$\boldsymbol{\Delta}\boldsymbol{\phi}_k = \lambda_k \boldsymbol{\phi}_k, \qquad k = 1, 2, \ldots$$

  - Eigenvectors are real and orthonormal (due to self-adjointness) $\langle \phi_k, \phi_{k'} \rangle_{L^2(\mathcal{V})} = \delta_{kk'}$
  - Eigenvalues are non-negative (due to positive-semidefiniteness) $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$

- Eigendecomposition of a graph Laplacian

$$\boldsymbol{\Delta} = \boldsymbol{\Phi}^T \boldsymbol{\Lambda} \boldsymbol{\Phi}$$

$$\text{where } \boldsymbol{\Phi} = (\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_n) \text{ and } \boldsymbol{\Lambda} = \text{diag}(\lambda_1, \ldots, \lambda_n)$$

Interpretation

- Find the smoothest orthonormal basis $\mathbf{\Phi} = (\boldsymbol{\phi}_1, \dots, \boldsymbol{\phi}_n)$ on a graph

$$\min_{\boldsymbol{\phi}_k} E_{\text{Dir}}(\boldsymbol{\phi}_k) \quad \text{s.t.} \quad \|\boldsymbol{\phi}_k\| = 1, \quad k = 2, 3, \dots n$$
$$\boldsymbol{\phi}_k \perp \text{span}\{\boldsymbol{\phi}_1, \dots, \boldsymbol{\phi}_{k-1}\}$$

where E_{Dir} is the Dirichlet energy = measure of smoothness of a function

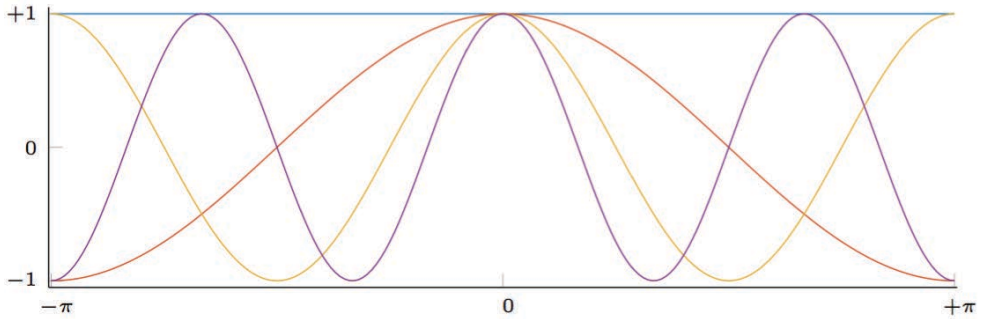
$$E_{\text{Dir}}(\mathbf{f}) = \mathbf{f}^\top \mathbf{\Delta} \mathbf{f}$$

- Solution: first n Laplacian eigenvectors

$$\min_{\mathbf{\Phi} \in \mathbb{R}^{n \times n}} \underbrace{\text{trace}(\mathbf{\Phi}^\top \mathbf{\Delta} \mathbf{\Phi})}_{\|\mathbf{\Phi}\|_{\mathcal{G}} \text{ Dirichlet norm}} \quad \text{s.t.} \quad \mathbf{\Phi}^\top \mathbf{\Phi} = \mathbf{I}$$

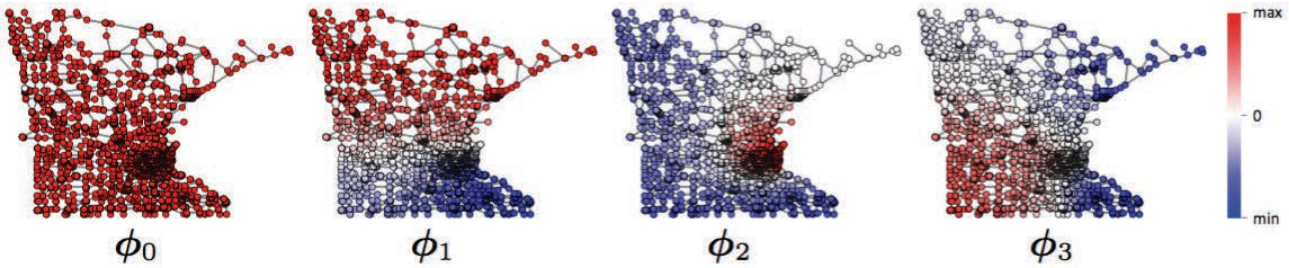
Laplacian eigenvectors

- Euclidean domain:



First eigenvectors of 1D Euclidean Laplacian = standard Fourier basis

- Graph domain:



First Laplacian eigenvectors of a graph

Lap eigenvectors related to graph geometry
(s.a. communities, hubs, etc), spectral clustering[10]

[10] Von Luxburg 2007

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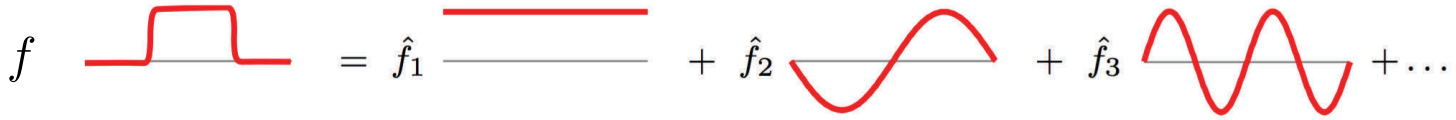
Fourier analysis on Euclidean spaces

- **A function** $f : [-\pi, \pi] \to \mathbb{R}$ **can be written as** Fourier series

$$f(x) = \sum_{k \geq 0} \underbrace{\frac{1}{2\pi} \int_{-\pi}^{\pi} f(x') e^{-ikx'} \, dx'}_{\hat{f}_k = \langle f, e^{-ikx} \rangle_{L^2([-\pi,\pi])}} e^{-ikx}$$



- **Fourier basis** e^{-ikx} = Laplace-Beltrami eigenfunctions:

$$-\Delta \phi_k = k^2 \phi_k$$

$$\begin{array}{rcl} \phi_k & = & \text{Fourier mode} \\ k & = & \text{frequency of Fourier mode} \end{array}$$

Fourier analysis on graphs[11]

- A function $f : \mathcal{V} \to \mathbb{R}$ can be written as Fourier series

$$f_i = \sum_{k=1}^{n} \underbrace{\langle f, \phi_k \rangle_{L^2(\mathcal{V})}}_{\hat{f}_k} \phi_{k,i}$$

- $\hat{f}_k$ is the k-th graph Fourier coefficient.
- In matrix-vector notation, with the n x n Fourier matrix $\mathbf{\Phi} = [\phi_1, ..., \phi_n]$

$$\hat{\mathbf{f}} = \mathbf{\Phi}^\top \mathbf{f} \quad \text{and} \quad \mathbf{f} = \mathbf{\Phi}\hat{\mathbf{f}}$$

Fourier transform

Inverse Fourier transform

- Graph Fourier basis ϕ_k = Laplacian eigenvectors :

$$\mathbf{\Delta}\phi_k = \lambda_k \phi_k$$

ϕ_k = graph Fourier mode

λ_k = (square) frequency

[11] Hammond, Vandergheynst, Gribonval, 2011

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Convolution on Euclidean spaces

- Given two functions $f, g : [-\pi, \pi] \to \mathbb{R}$ their convolution is a function

$$(f \star g)(x) = \int_{-\pi}^{\pi} f(x')g(x - x')dx'$$

  - Shift-invariance: $f(x - x_0) \star g(x) = (f \star g)(x - x_0)$
  - Convolution operator commutes with Laplacian: $(\Delta f) \star g = \Delta(f \star g)$
  - Convolution theorem: Convolution can be computed in the Fourier domain as

$$\widehat{(f \star g)} = \hat{f} \cdot \hat{g}$$

  - Efficient computation using FFT: $O(n \log n)$

Convolution on discrete Euclidean spaces

- **Convolution of two vectors** $\mathbf{f} = (f_1, \dots, f_n)^\top$ and $\mathbf{g} = (g_1, \dots, g_n)^\top$

$$(\mathbf{f} \star \mathbf{g})_i = \sum_m g_{(i-m) \bmod n} \cdot f_m$$

$$\mathbf{f} \star \mathbf{g} = \underbrace{\begin{bmatrix} g_1 & g_2 & \cdots & \cdots & g_n \\ g_n & g_1 & g_2 & \cdots & g_{n-1} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ g_3 & g_4 & \cdots & g_1 & g_2 \\ g_2 & g_3 & \cdots & \cdots & g_1 \end{bmatrix}}_{\text{Circulant matrix}} \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}$$

diagonalised by Fourier basis (Toeplitz)

$$= \mathbf{\Phi} \begin{bmatrix} \hat{g}_1 & & \\ & \ddots & \\ & & \hat{g}_n \end{bmatrix} \mathbf{\Phi}^\top \mathbf{f} = \mathbf{\Phi}\left(\mathbf{\Phi}^\top \mathbf{g} \circ \mathbf{\Phi}^\top \mathbf{f}\right)$$

Convolution on graphs[11]

- Spectral convolution of $f, g \in L^2(\mathcal{V})$ can be defined by analogy

$$(f \star g)_i = \underbrace{\sum_{k \geq 1} \underbrace{\langle f, \phi_k \rangle_{L^2(\mathcal{V})} \langle g, \phi_k \rangle_{L^2(\mathcal{V})}}_{\text{product in the Fourier domain}} \phi_{k,i}}_{\text{inverse Fourier transform}}$$

- In matrix-vector notation

$$\begin{aligned} \mathbf{f} \star \mathbf{g} &= \boldsymbol{\Phi} (\boldsymbol{\Phi}^\top \mathbf{g} \circ \boldsymbol{\Phi}^\top \mathbf{f}) \\ &= \underbrace{\boldsymbol{\Phi} \operatorname{diag}(\hat{g}_1, \dots, \hat{g}_n) \boldsymbol{\Phi}^\top}_{\mathbf{G}} \mathbf{f} \\ &= \boldsymbol{\Phi} \hat{g}(\boldsymbol{\Lambda}) \boldsymbol{\Phi}^\top \mathbf{f} = \hat{g}(\boldsymbol{\Phi} \boldsymbol{\Lambda} \boldsymbol{\Phi}^\top) \mathbf{f} = \hat{g}(\boldsymbol{\Delta}) \mathbf{f} \end{aligned}$$

  - Not shift-invariant! (G has no circulant structure)
  - Commutes with Laplacian: $\mathbf{G}\boldsymbol{\Delta}\mathbf{f} = \boldsymbol{\Delta}\mathbf{G}\mathbf{f}$
  - Filter coefficients depend on basis $\phi_1, \dots, \phi_n$
  - Expensive computation (no FFT): $O(n^2)$

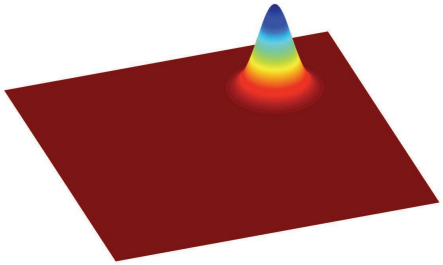
[11] Hammond, Vandergheynst, Gribonval, 2011

No shift invariance on graphs

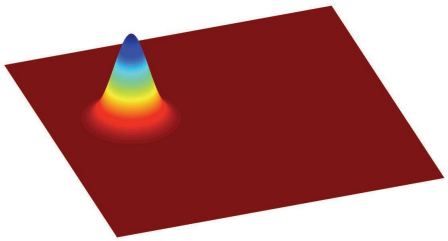
- A signal f on graph can be translated to vertex i:

$$T_i \mathbf{f} = \mathbf{f} \star \boldsymbol{\delta}_i$$

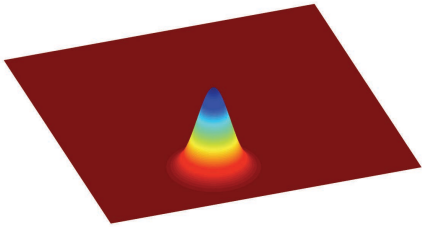
- Euclidean domain



(a) $T_s f$

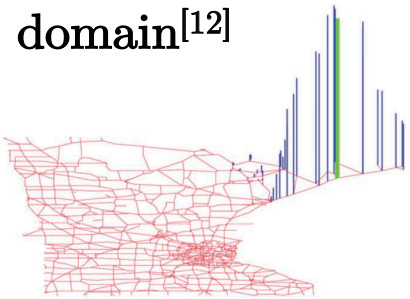


(b) $T_{s'} f$

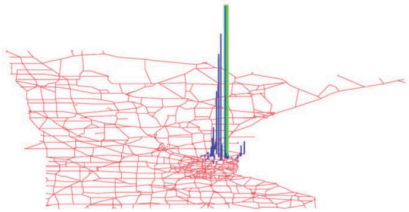


(c) $T_{s''} f$

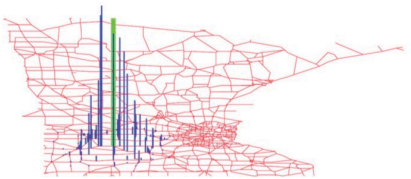
- Graph domain[12]



(d) $T_i f$



(e) $T_{i'} f$



(f) $T_{i''} f$

[12] Shuman et al. 2016

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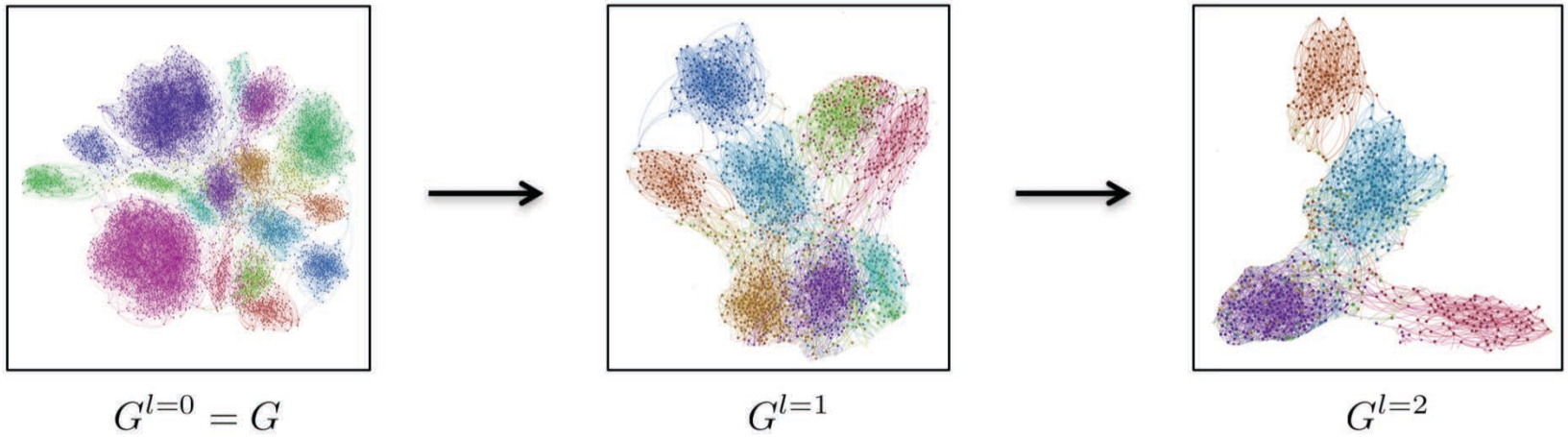
Graph coarsening for graph pooling

- Goals:
  - Pool similar local features (max pooling).
  - Series of pooling layers create invariance to global geometric deformations.

- Challenges:
  - Design a multi-scale coarsening algorithm that preserves non-linear graph structures.
  - How to make graph pooling fast?

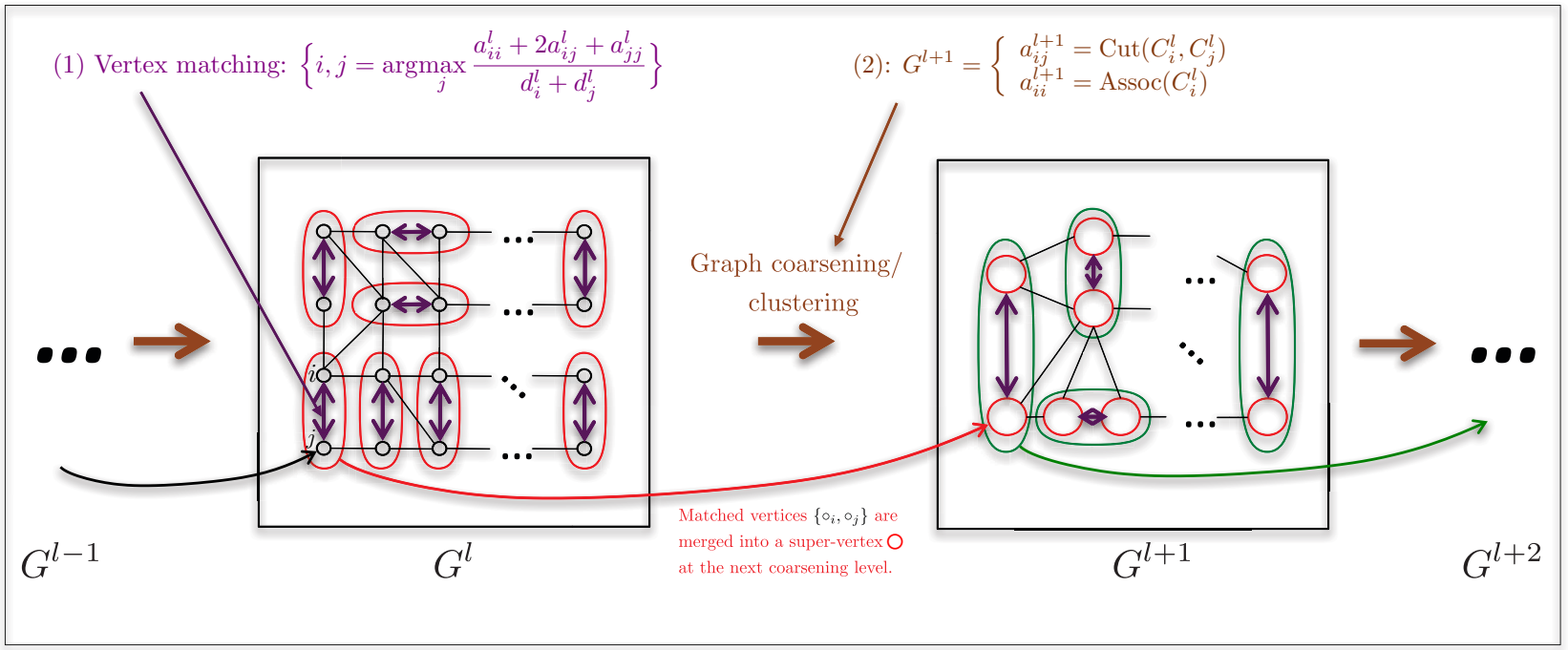
Graph coarsening = graph partitioning



- Graph partitioning decomposes G into smaller meaningful clusters.
- NP-hard ⇒ Approximation

Coarsening with Heavy-Edge Matching

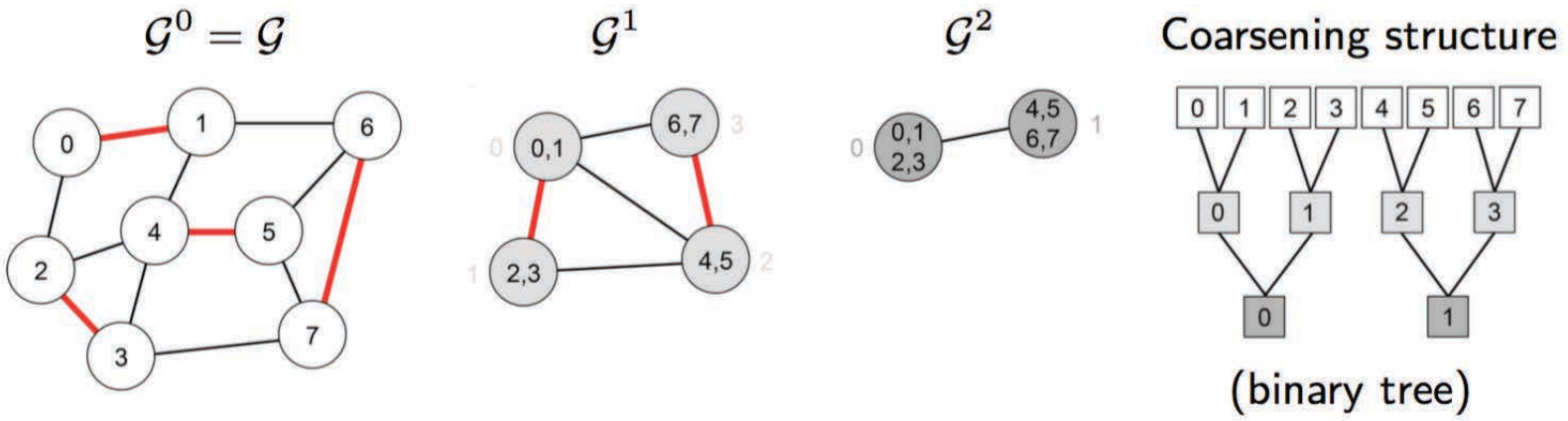
- **HEM proceeds by two successive steps, vertex matching and graph coarsening (that guarantees a local solution of Norm assoc):**



[14] Dhillon, Guan, Kulis 2007
[15] Karypis, Kumar 1995

Fast graph pooling[18]

- **Structured pooling:** Arrangement of the node indexing such that adjacent nodes are hierarchically merged at the next coarser level.



☺ As efficient as 1D-Euclidean grid pooling.

[18] Defferrard, Bresson, Vandergheynst 2016

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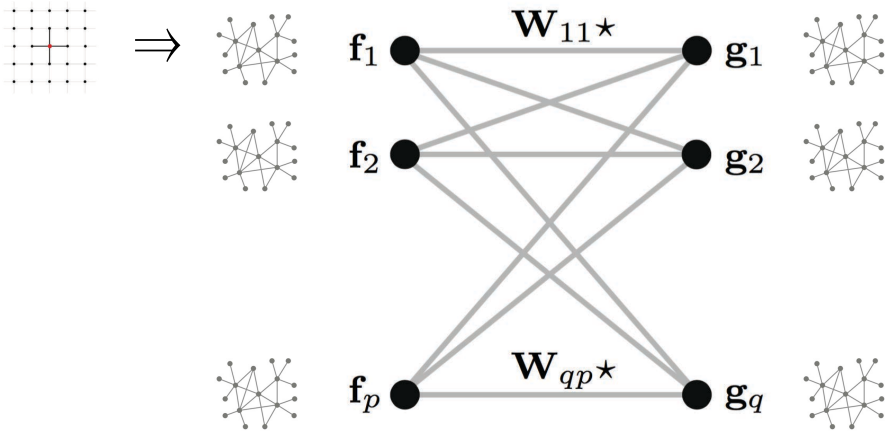
Vanilla spectral graph ConvNets[16]

- Graph convolutional layer

$$\begin{aligned} \mathbf{f}_l &= l\text{-th data feature on graphs, } \dim(\mathbf{f}_l) = n \times 1 \\ \mathbf{g}_l &= l\text{-th feature map, } \dim(\mathbf{g}_l) = n \times 1 \end{aligned}$$



Conv. layer $\quad \mathbf{g}_l = \xi\left(\sum_{l'=1}^{p} \mathbf{W}_{l,l'} \star \mathbf{f}_{l'}\right)$

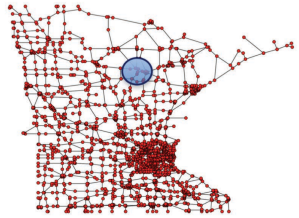
Activation, e.g. $\quad \xi(x) = \max\{x, 0\}$ $\quad$ rectified linear unit (ReLU)

[16] Bruna, Zaremba, Szlam, LeCun 2014

Spectral graph convolution

- Convolutional layer in the spatial domain:

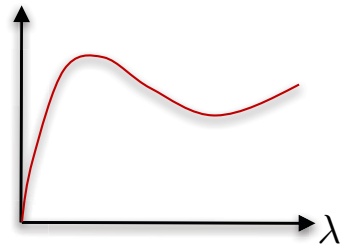
$$\mathbf{g}_l = \xi\left(\sum_{l'=1}^{p} \mathbf{W}_{l,l'} \star \mathbf{f}_{l'}\right),$$



where $\mathbf{W}_{l,l'}$ = matrix of graph spatial filter,

can also be expressed in the spectral domain (using $\mathbf{g} \star \mathbf{f} = \mathbf{\Phi}\, \hat{g}(\mathbf{\Lambda})\mathbf{\Phi}^\top \mathbf{f}$)

$$\mathbf{g}_l = \xi\left(\sum_{l'=1}^{p} \mathbf{\Phi}\hat{\mathbf{W}}_{l,l'}\mathbf{\Phi}^\top \mathbf{f}_{l'}\right),$$



where $\hat{\mathbf{W}}_{l,l'}$ = n x n diagonal matrix of graph spectral filter.

We will denote the spectral filter without the hat symbol, i.e. $\mathbf{W}_{l,l'}$

Vanilla spectral graph ConvNets[16]

- Series of spectral convolutional layers

$$\mathbf{g}_l^{(k)} = \xi\left(\sum_{l'=1}^{q^{(k-1)}} \mathbf{\Phi}\mathbf{W}_{l,l'}^{(k)}\mathbf{\Phi}^\top \mathbf{g}_{l'}^{(k-1)}\right),$$

with spectral coefficients $\mathbf{W}_{l,l'}^{(k)}$ to be learned at each layer.

☺ First spectral graph CNN architecture

☹ No guarantee of spatial localization of filters

☹ $O(n)$ parameters per layer

☹ $O(n^2)$ computation of forward and inverse Fourier transforms $\phi, \phi^\top$ (no FFT on graphs)

☹ Filters are basis-dependent ⇒ does not generalize across graphs

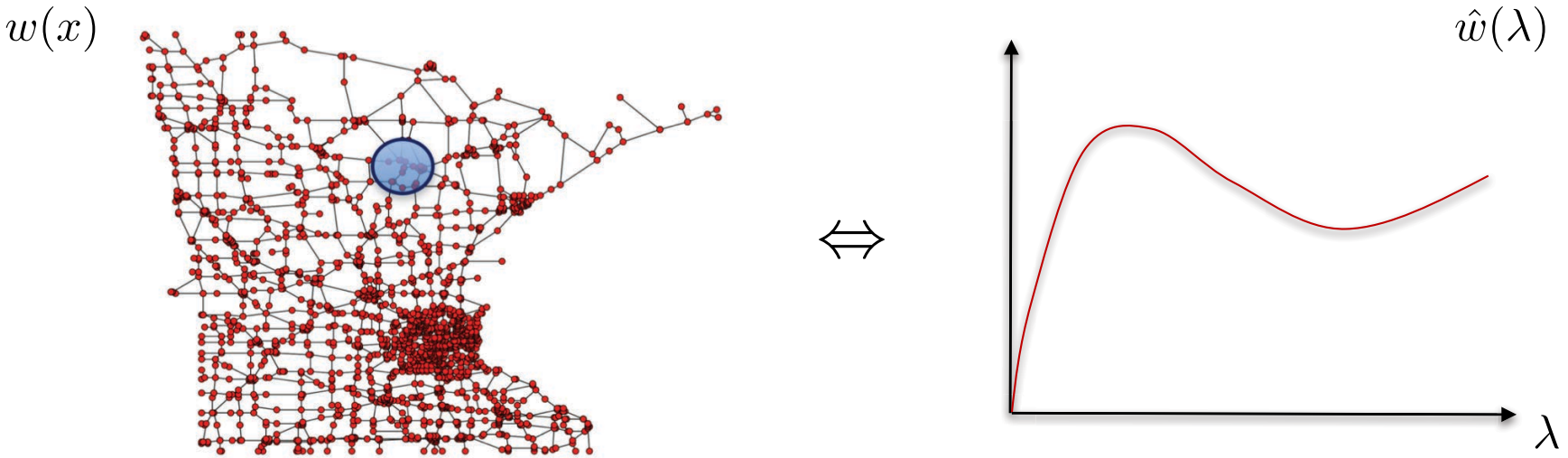
[16] Bruna, Zaremba, Szlam, LeCun 2014

Spatial localization and spectral smoothness[17]

- In the Euclidean setting (by Parseval's identity)

$$\int_{-\infty}^{+\infty} |x|^{2k} |w(x)|^2 dx = \int_{-\infty}^{+\infty} \left| \frac{\partial^k \hat{w}(\lambda)}{\partial \lambda^k} \right|^2 d\lambda$$

$\Rightarrow$ Localization in space = smoothness in frequency domain



Spatial localization

Smooth spectral filter function

[17] Henaff, Bruna, LeCun 2015

Smooth parametric spectral filter

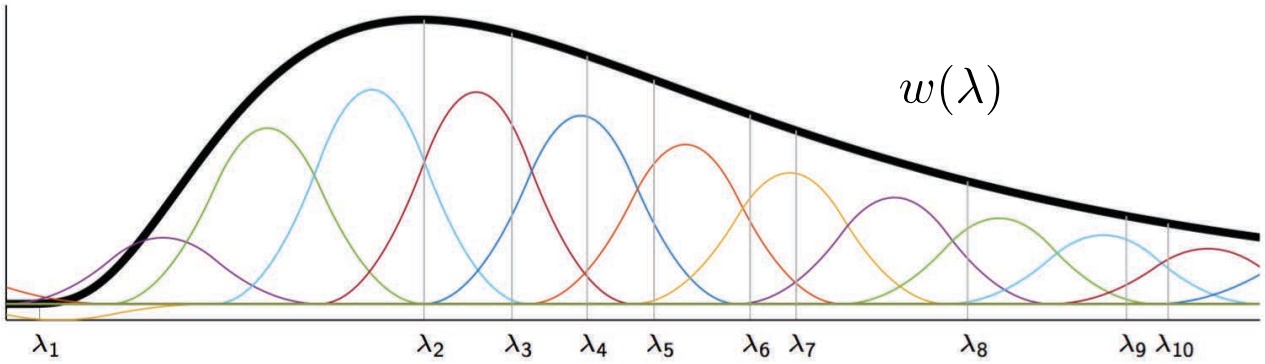
- **Parametrize the smooth spectral filter function $w_(\lambda)$ with a linear combination of smooth kernel functions $\beta_1(\lambda), \ldots, \beta_r(\lambda)$, e.g. splines[17]**

$$w_{\boldsymbol{\alpha}}(\lambda) = \sum_{j=1}^{r} \alpha_j \beta_j(\lambda)$$

$$\Downarrow$$

$$w_{\boldsymbol{\alpha}}(\lambda_i) = \sum_{j=1}^{r} \alpha_j \beta_j(\lambda_i) = (\mathbf{B}\boldsymbol{\alpha})_i \quad \Longrightarrow \quad \mathbf{W} = \mathrm{Diag}(\mathbf{B}\boldsymbol{\alpha})$$

where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_r)^\top$ is the vector of filter parameters



[17] (Litman, Bronstein, 2014); Henaff, Bruna, LeCun 2015

SplineNets[17]

- Series of spectral convolutional layers

$$\mathbf{g}_l^{(k)} = \xi\left(\sum_{l'=1}^{q^{(k-1)}} \mathbf{\Phi}\mathbf{W}_{l,l'}^{(k)}\mathbf{\Phi}^\top \mathbf{g}_{l'}^{(k-1)}\right),$$

with smooth spectral parametric coefficients $\mathbf{W}_{l,l'}^{(k)}$ to be learned at each layer.

- ☺ Fast-decaying filters in space
- ☺ O(1) parameters per layer
- ☹ $O(n^2)$ computation of forward and inverse Fourier transforms $\phi, \phi^\top$ (no FFT on graphs)
- ☹ Filters are basis-dependent ⇒ does not generalize across graphs

[17] Henaff, Bruna, LeCun 2015

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Spectral polynomial filters[18]

- Represent smooth spectral functions with polynomials of Laplacian eigenvalues

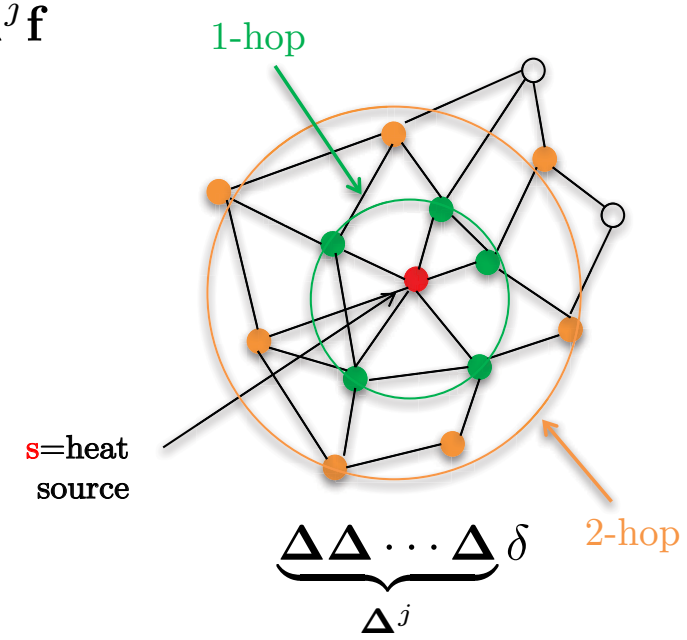
$$w_{\boldsymbol{\alpha}}(\lambda) = \sum_{j=0}^{r} \alpha_j \lambda^j$$

where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_r)^\top$ is the vector of filter parameters.

- Convolutional layer: Apply spectral filter to feature signal f

$$w_{\boldsymbol{\alpha}}(\boldsymbol{\Delta})\mathbf{f} = \textstyle\sum_{j=0}^{r} \alpha_j \boldsymbol{\Delta}^j \mathbf{f}$$

- Key observation: Each Laplacian operation increases the support of a function by 1-hop ⇒ Exact control the size of Laplacian-based filters.



[18] Defferrard, Bresson, Vandergheynst 2016

Linear complexity

- Application of the filter to a feature signal f

$$w_{\boldsymbol{\alpha}}(\boldsymbol{\Delta})\mathbf{f} = \sum_{j=0}^{r} \alpha_j \boldsymbol{\Delta}^j \mathbf{f}$$

- Denote $\mathbf{X}_0 = \mathbf{f}$ and define $\mathbf{X}_1 = \boldsymbol{\Delta}\mathbf{X}_0 = \boldsymbol{\Delta}\mathbf{f}$ and the sequence $\mathbf{X}_j = \boldsymbol{\Delta}\mathbf{X}_{j-1}$

$$w_{\boldsymbol{\alpha}}(\boldsymbol{\Delta})\mathbf{f} = \sum_{j=0}^{r} \alpha_j \mathbf{X}_j$$

- Two important observations:

  1. *No* need to compute the eigendecomposition of the Laplacian (ϕ,Λ).

  2. Observe that $\{X_j\}$ are generated by multiplication of a sparse matrix and a vector $\Rightarrow$ Complexity is $O(Er)$=$O(n)$ for sparse graphs.

- Graph convolutional layers are GPU friendly.

Spectral graph ConvNets with polynomial filters

- Series of spectral convolutional layers

$$\mathbf{g}_l^{(k)} = \xi\left(\sum_{l'=1}^{q^{(k-1)}} \mathbf{\Phi}\mathbf{W}_{l,l'}^{(k)}\mathbf{\Phi}^\top \mathbf{g}_{l'}^{(k-1)}\right),$$

with spectral polynomial coefficients $\mathbf{W}_{l,l'}^{(k)}$ to be learned at each layer.

- ☺ Filters are exactly localized in r-hops support
- ☺ O(1) parameters per layer
- ☺ No computation of ϕ, $\phi^\top \Rightarrow$ O(n) computational complexity (assuming sparsely-connected graphs)
- ☹ Unstable under coefficients perturbation (hard to optimize)
- ☹ Filters are basis-dependent $\Rightarrow$ does not generalize across graphs

[18] Defferrard, Bresson, Vandergheynst 2016

Chebyshev polynomials

- Graph convolution with (non-orthogonal) monomial basis $1, x, x^2, x^3, \cdots$

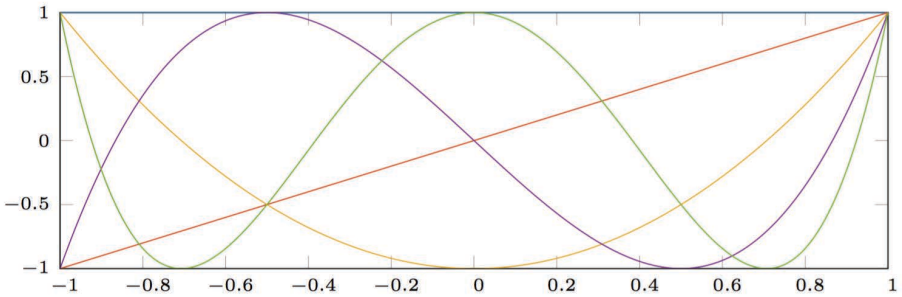
$$w_{\boldsymbol{\alpha}}(\boldsymbol{\Delta})\mathbf{f} = \sum_{j=0}^{r} \alpha_j \boldsymbol{\Delta}^j \mathbf{f}$$

- Graph convolution with (orthogonal) Chebyshev polynomials

$$w_{\boldsymbol{\alpha}}(\tilde{\boldsymbol{\Delta}})\mathbf{f} = \sum_{j=0}^{r} \alpha_j T_j(\tilde{\boldsymbol{\Delta}})\mathbf{f}$$

- Orthonormal on $L^2([-1,+1])$ w.r.t. $\langle f, g \rangle = \int_{-1}^{+1} f(\tilde{\lambda}) g(\tilde{\lambda}) \frac{d\tilde{\lambda}}{\sqrt{1-\tilde{\lambda}^2}}$

- Stable under perturbation of coefficients



T_0, T_1, T_2, T_3

ChebNets[18]

- Application of the filter with the scaled Laplacian $\tilde{\mathbf{\Delta}} = 2\lambda_n^{-1}\mathbf{\Delta} - \mathbf{I}$

$$w_{\boldsymbol{\alpha}}(\tilde{\mathbf{\Delta}})\mathbf{f} = \sum_{j=0}^{r} \alpha_j T_j(\tilde{\mathbf{\Delta}})\mathbf{f} = \sum_{j=0}^{r} \alpha_j \mathbf{X}^{(j)}$$

with

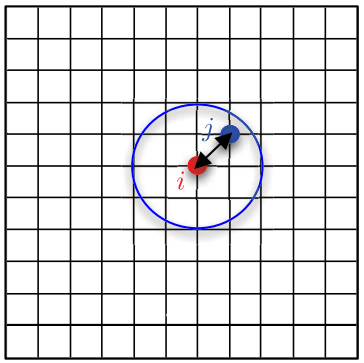
$$\begin{aligned} \mathbf{X}^{(j)} &= T_j(\tilde{\mathbf{\Delta}})\mathbf{f} \\ &= 2\tilde{\mathbf{\Delta}}\mathbf{X}^{(j-1)} - \mathbf{X}^{(j-2)}, \qquad \mathbf{X}^{(0)} = \mathbf{f}, \quad \mathbf{X}^{(1)} = \tilde{\mathbf{\Delta}}\mathbf{f} \end{aligned}$$

- ☺ Filters are exactly localized in r-hops support
- ☺ O(1) parameters per layer
- ☺ No computation of ϕ, $\phi^\intercal \Rightarrow$ O(n) computational complexity (assuming sparsely-connected graphs)
- ☺ Stable under coefficients perturbation
- ☹ Filters are basis-dependent $\Rightarrow$ does not generalize across graphs

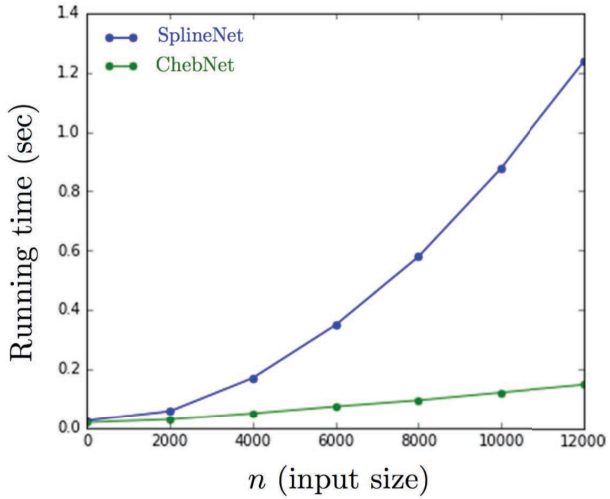
[18] Defferrard, Bresson, Vandergheynst 2016

Numerical experiments

Graph: a 8-NN graph of the Euclidean grid



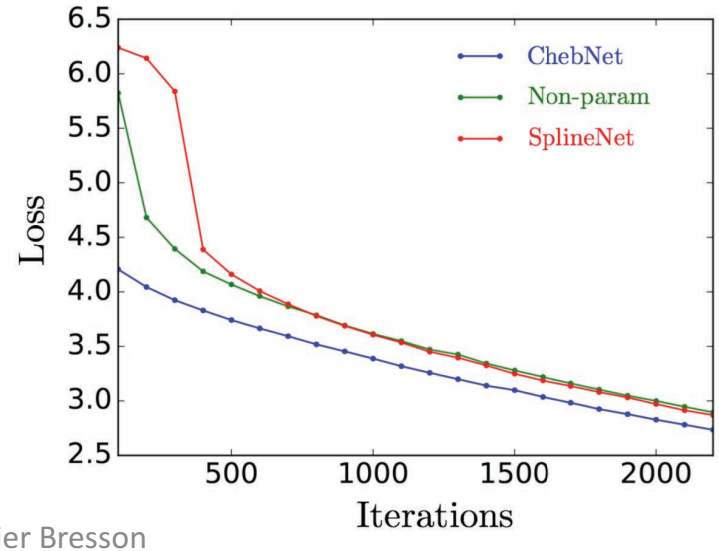
- Running time

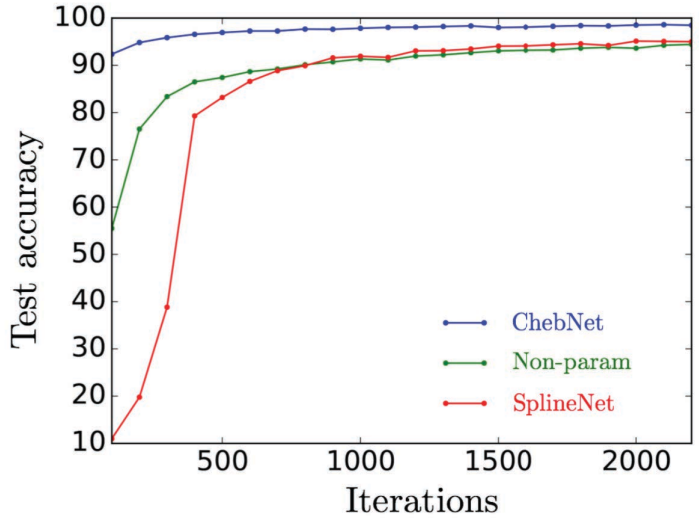


- Accuracy

Model	Order	Accuracy
LeNet5	-	99.33%
SplineNet	25	97.75%
ChebNet	25	99.14%

- Optimization





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Graph convolutional nets[19]: simplified ChebNets

- Use Chebychev polynomials of degree $r=2$ and assume $\lambda_n \approx 2$

$$\begin{aligned} w_{\boldsymbol{\alpha}}(\boldsymbol{\Delta})\mathbf{f} &= \alpha_0\mathbf{f} + \alpha_1(\boldsymbol{\Delta} - \mathbf{I})\mathbf{f} \\ &= \alpha_0\mathbf{f} - \alpha_1\mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}\mathbf{f} \end{aligned}$$

- Further constrain $\alpha = \alpha_0 = -\alpha_1$ to obtain a single-parameter filter

$$w_\alpha(\boldsymbol{\Delta})\mathbf{f} = \alpha(\mathbf{I} + \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2})\mathbf{f}$$

- Caveat: The eigenvalues of $\mathbf{I} + \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}$ are now in [0,2]

  $\Rightarrow$ repeated application of the filter results in numerical instability

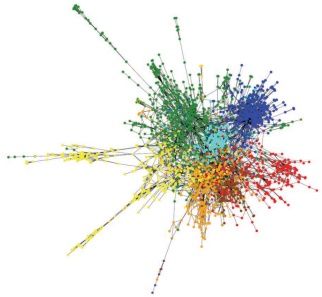
- Fix: Apply a renormalization

$$w_\alpha(\boldsymbol{\Delta})\mathbf{f} = \alpha\tilde{\mathbf{D}}^{-1/2}\tilde{\mathbf{W}}\tilde{\mathbf{D}}^{-1/2}\mathbf{f}$$

$$\text{with } \tilde{\mathbf{W}} = \mathbf{W} + \mathbf{I} \text{ and } \tilde{\mathbf{D}} = \text{diag}(\textstyle\sum_{j\neq i} \tilde{w}_{ij})$$

[19] Kipf, Welling 2016

Example: citation networks



Method	Cora[1]	PubMed[2]
Manifold Regularization[3]	59.5%	70.7%
Semidefinite Embedding[4]	59.0%	71.1%
Label Propagation[5]	68.0%	63.0%
DeepWalk[6]	67.2%	65.3%
Planetoid[7]	75.7%	77.2%
Graph Convolutional Net[8]	**81.59%**	**78.72%**

Classification accuracy of different methods on citation network datasets

Monti et al. 2016; data: [1,2]Sen et al. 2008; methods: [3]Belkin et al. 2006; [4]Weston et al. 2012; [5]Zhu et al. 2003; [6]Perozzi et al. 2014; [7]Yang et al. 2016; [8]Kipf, Welling 2016

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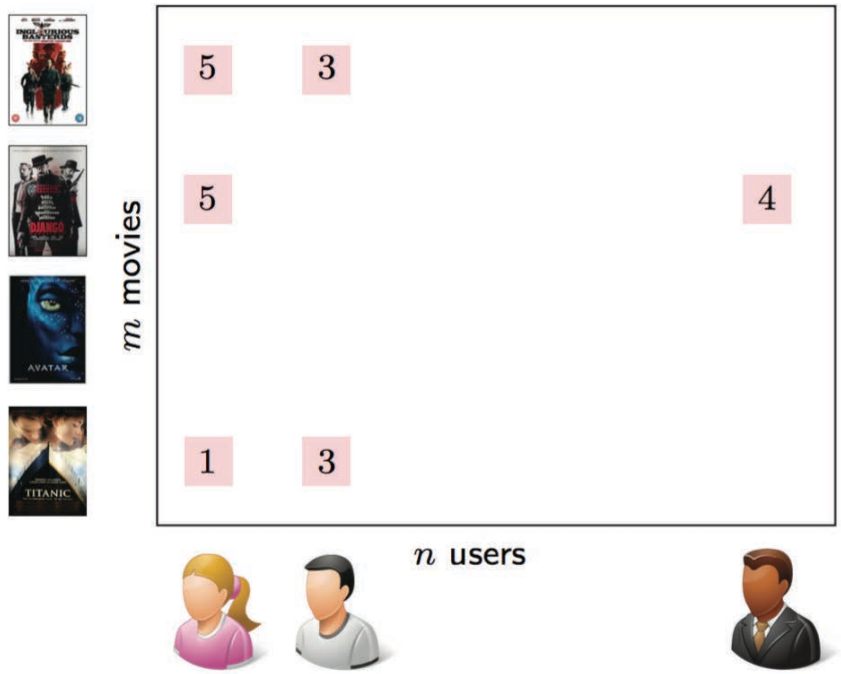
Matrix completion - Netflix challenge



$$\min_{\mathbf{X}\in\mathbb{R}^{m\times n}} \quad \text{rank}(\mathbf{X}) \quad \text{s.t.} \quad x_{ij} = a_{ij} \;\; \forall ij \in \Omega$$

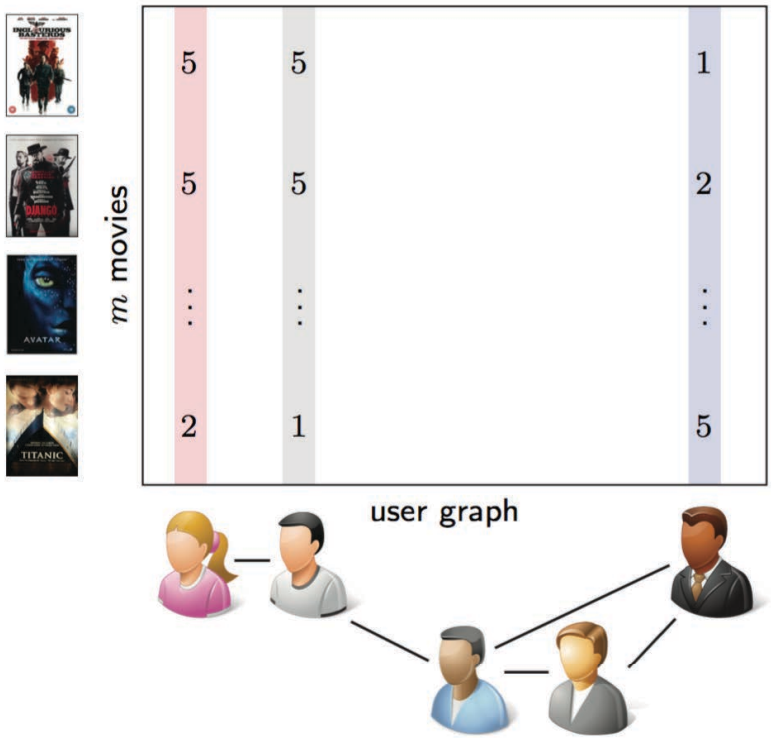
$$\Downarrow \text{ Convex relaxation}^{[21]}$$

$$\min_{\mathbf{X}\in\mathbb{R}^{m\times n}} \quad \|\mathbf{X}\|_* \quad \text{s.t.} \quad x_{ij} = a_{ij} \;\; \forall ij \in \Omega$$

$$\min_{\mathbf{X}\in\mathbb{R}^{m\times n}} \quad \|\mathbf{X}\|_* + \mu\|\mathbf{\Omega} \circ (\mathbf{X} - \mathbf{A})\|_{\text{F}}^2$$

[21] Candes et al. 2008

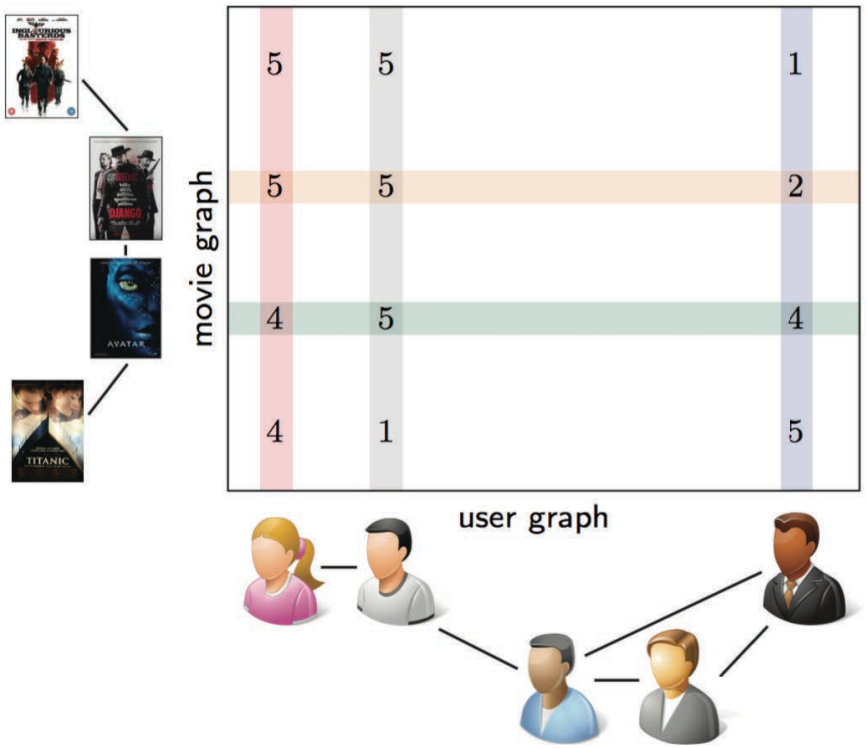
Matrix completion on single graph[22]



$$\min_{\mathbf{X}\in\mathbb{R}^{m\times n}} \quad \|\mathbf{X}\|_* + \mu\|\boldsymbol{\Omega}\circ(\mathbf{X}-\mathbf{A})\|_{\mathrm{F}}^2 + \mu_{\mathrm{c}}\underbrace{\mathrm{tr}(\mathbf{X}\boldsymbol{\Delta}_{\mathrm{c}}\mathbf{X}^\top)}_{\|\mathbf{X}\|_{\mathcal{G}_{\mathrm{c}}}^2}$$

[22] Kalofolias, Bresson, Bronstein, Vandergheynst, 2014

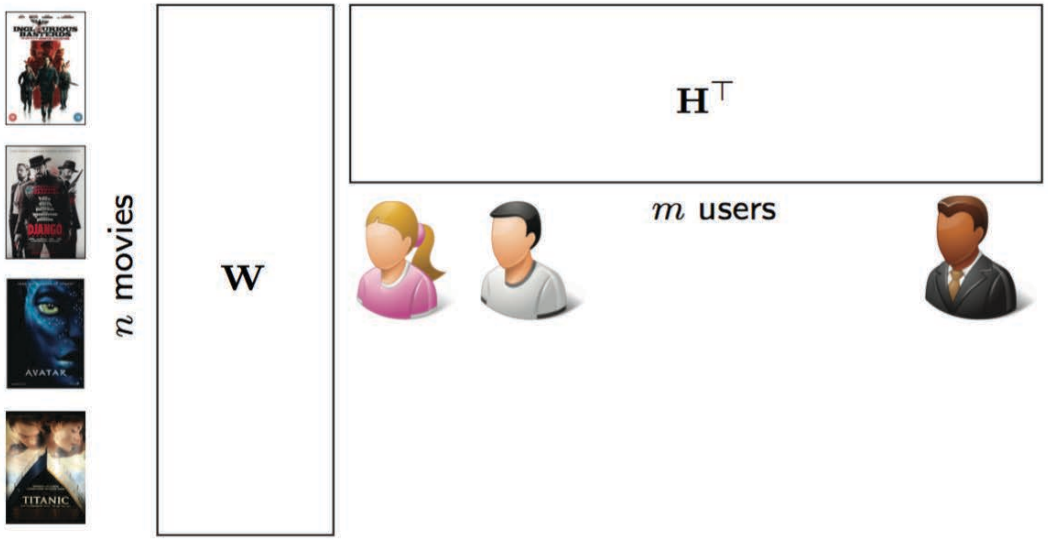
Matrix completion on multiple graphs[22]



$$\min_{\mathbf{X}\in\mathbb{R}^{m\times n}} \quad \|\mathbf{X}\|_* + \mu\|\mathbf{\Omega}\circ(\mathbf{X}-\mathbf{A})\|_{\mathrm{F}}^2 + \mu_{\mathrm{c}}\underbrace{\mathrm{tr}(\mathbf{X}\mathbf{\Delta}_{\mathrm{c}}\mathbf{X}^\top)}_{\|\mathbf{X}\|_{\mathcal{G}_{\mathrm{c}}}^2} + \mu_{\mathrm{r}}\underbrace{\mathrm{tr}(\mathbf{X}^\top\mathbf{\Delta}_{\mathrm{r}}\mathbf{X})}_{\|\mathbf{X}\|_{\mathcal{G}_{\mathrm{r}}}^2}$$

[22] Kalofolias, Bresson, Bronstein, Vandergheynst, 2014

Factorized matrix completion models[23]



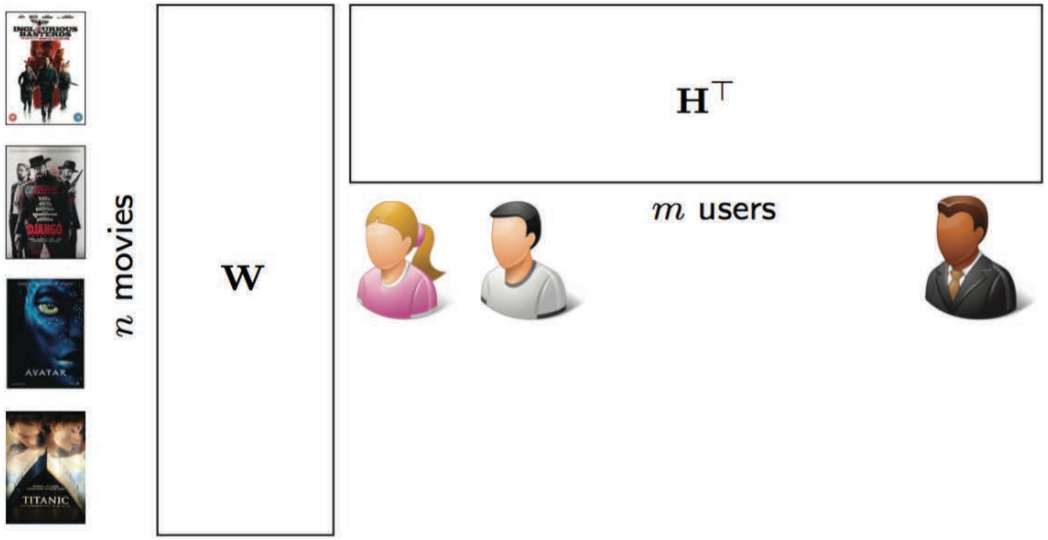
$$\min_{\substack{\mathbf{W}\in\mathbb{R}^{m\times s}\\ \mathbf{H}\in\mathbb{R}^{n\times s}}} \mu\|\mathbf{\Omega}\circ(\mathbf{X}-\mathbf{A})\|_{\mathrm{F}}^2+\mu_{\mathrm{c}}\|\mathbf{W}\|_{\mathrm{F}}^2+\mu_{\mathrm{r}}\|\mathbf{H}\|_{\mathrm{F}}^2$$

☺ O(n+m) variables instead of O(nm)

☺ rank(X) = rank(WH$^{\mathrm{T}}$) ≤ s by construction

[23] Srebro, Rennie, Jaakkola 2004

Factorized matrix completion on graphs[24]



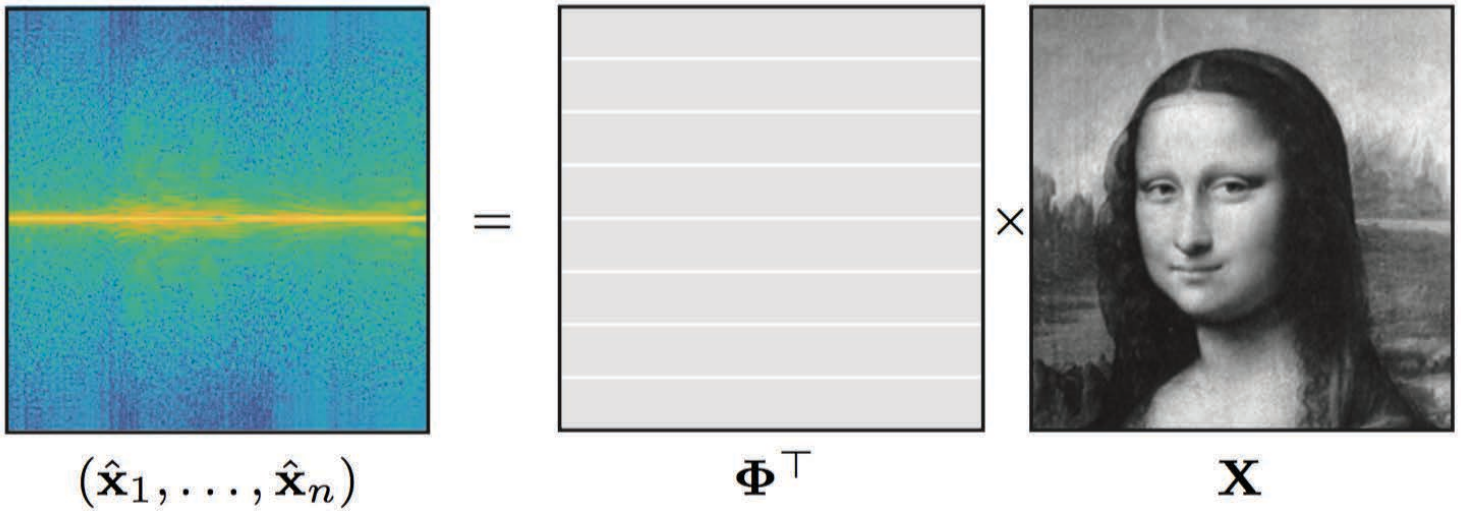
$$\min_{\substack{\mathbf{W}\in\mathbb{R}^{m\times s}\\ \mathbf{H}\in\mathbb{R}^{n\times s}}} \quad \mu\|\mathbf{\Omega}\circ(\mathbf{X}-\mathbf{A})\|_{\mathrm{F}}^2+\mu_{\mathrm{c}}\mathrm{tr}(\mathbf{H}^\top\mathbf{\Delta}_{\mathrm{c}}\mathbf{H})+\mu_{\mathrm{r}}\mathrm{tr}(\mathbf{W}^\top\mathbf{\Delta}_{\mathrm{r}}\mathbf{W})$$

☺ O(n+m) variables instead of O(nm)

☺ rank(X) = rank(WH$^{\mathrm{T}}$) ≤ s by construction

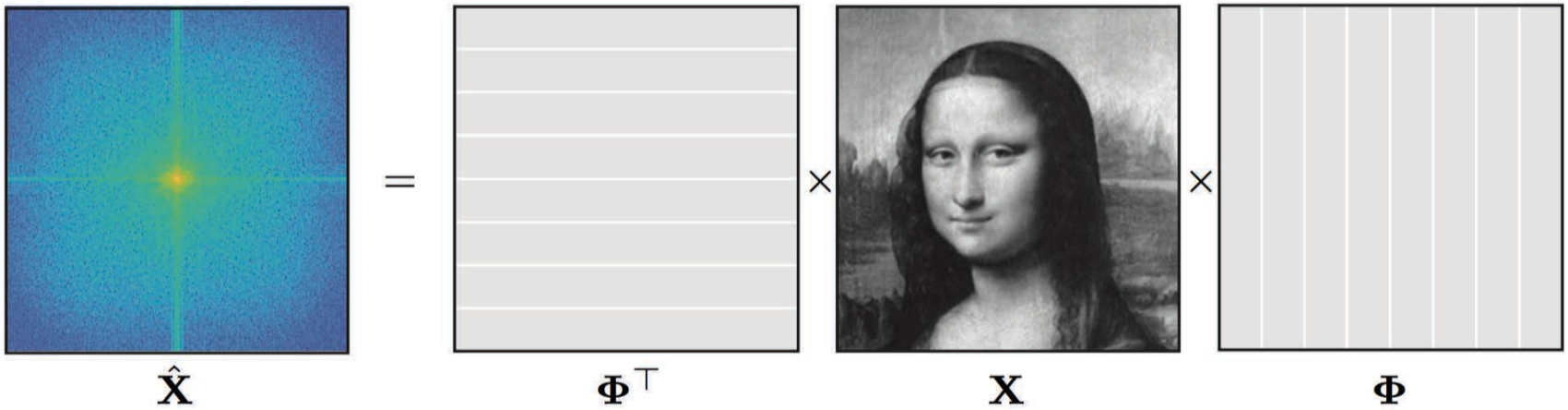
[24] Rao et al. 2015

1D Fourier transform



Column-wise transform

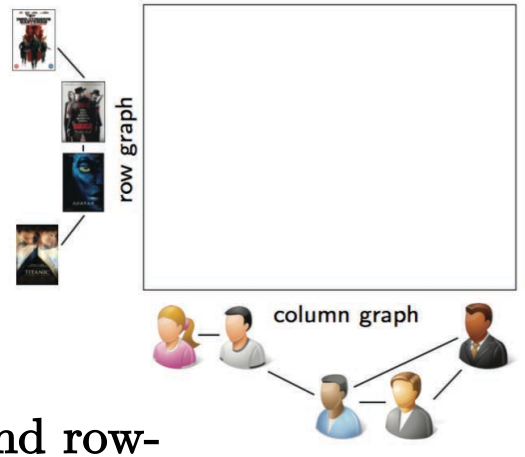
2D Fourier transform



Column-wise transform + Row-wise transform = 2D transform

From 1D signal processing to 2D image processing

Multi-graph Fourier transform and convolution[25]



- Multi-graph Fourier transform

$$\hat{\mathbf{X}} = \mathbf{\Phi}_{\mathrm{r}}^{\top} \mathbf{X} \mathbf{\Phi}_{\mathrm{c}}$$

where $\mathbf{\Phi}_{\mathrm{c}}$, $\mathbf{\Phi}_{\mathrm{r}}$ are the eigenvectors of the column- and row-graph Laplacians $\mathbf{\Delta}_{\mathrm{c}}$, $\mathbf{\Delta}_{\mathrm{r}}$, respectively.

- Multi-graph spectral convolution

$$\begin{aligned} \mathbf{X} \star \mathbf{Y} &= \mathbf{\Phi}_{\mathrm{r}}((\mathbf{\Phi}_{\mathrm{r}}^{\top} \mathbf{X} \mathbf{\Phi}_{\mathrm{c}}) \circ (\mathbf{\Phi}_{\mathrm{r}}^{\top} \mathbf{Y} \mathbf{\Phi}_{\mathrm{c}})) \mathbf{\Phi}_{\mathrm{c}}^{\top} \\ &= \mathbf{\Phi}_{\mathrm{r}}(\hat{\mathbf{X}} \circ \hat{\mathbf{Y}}) \mathbf{\Phi}_{\mathrm{c}}^{\top} \end{aligned}$$

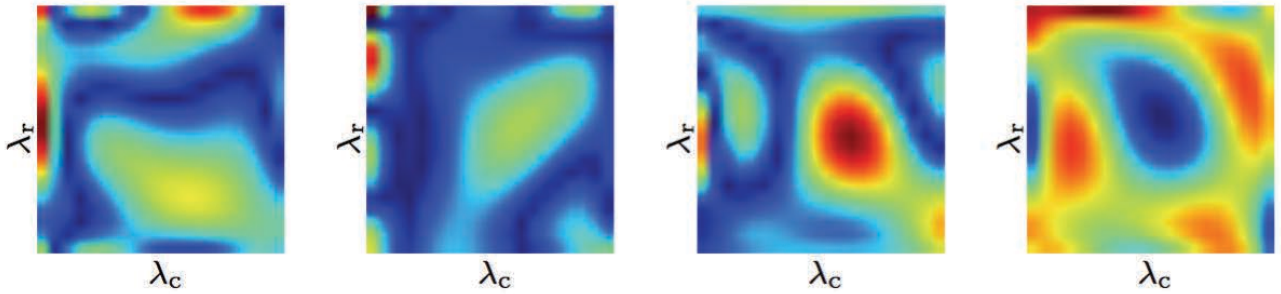
[25] Monti, Bresson, Bronstein 2017

Multi-graph spectral filters

- Parametrize the multi-graph filter as a smooth function of column- and row frequencies w/ e.g. bivariate Chebyshev polynomial

$$w_{\mathbf{\Theta}}(\tilde{\lambda}_{\mathrm{c}}, \tilde{\lambda}_{\mathrm{r}}) = \sum_{j,j'=1}^{r} \theta_{jj'} T_j(\tilde{\lambda}_{\mathrm{c}}) T_{j'}(\tilde{\lambda}_{\mathrm{r}})$$

where $\mathbf{\Theta} = (\theta_{jj'})$ is matrix of coefficients and $-1 \leq \tilde{\lambda}_{\mathrm{c}}, \tilde{\lambda}_{\mathrm{r}} \leq 1$



Examples of multi-graph spectral filters (shown is $|\tau(\tilde{\lambda}_{\mathrm{c}}, \tilde{\lambda}_{\mathrm{r}})|$)

- Multi-graph convolutional layer: Apply filter to matrix $\mathbf{X}$

$$\mathbf{Y} = \sum_{j,j'=1}^{r} \theta_{jj'} T_j(\tilde{\mathbf{\Delta}}_{\mathrm{c}}) \mathbf{X} T_{j'}(\tilde{\mathbf{\Delta}}_{\mathrm{r}})$$

where the scaled Laplacians $\tilde{\mathbf{\Delta}}_{\mathrm{c}} = 2\lambda_{\mathrm{c},n}^{-1} \mathbf{\Delta}_{\mathrm{c}} - \mathbf{I}$ and $\tilde{\mathbf{\Delta}}_{\mathrm{r}} = 2\lambda_{\mathrm{r},m}^{-1} \mathbf{\Delta}_{\mathrm{r}} - \mathbf{I}$

Multi-graph ConvNets[25]

- **Multi-graph spectral filters**

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

applied to p input channels (m x n matrices $\mathbf{Y}_1^{(k-1)},\dots,\mathbf{Y}_p^{(k-1)}$) and producing q output channels $\mathbf{Y}_1^{(k)},\dots,\mathbf{Y}_q^{(k)}$

☺ Filters have guaranteed r-hops support on both graphs

☺ O(1) parameters per layer

☹ O(nm) computational complexity (assuming sparse graphs)

[25] Monti, Bresson, Bronstein 2017

Factorized multi-graph ConvNets

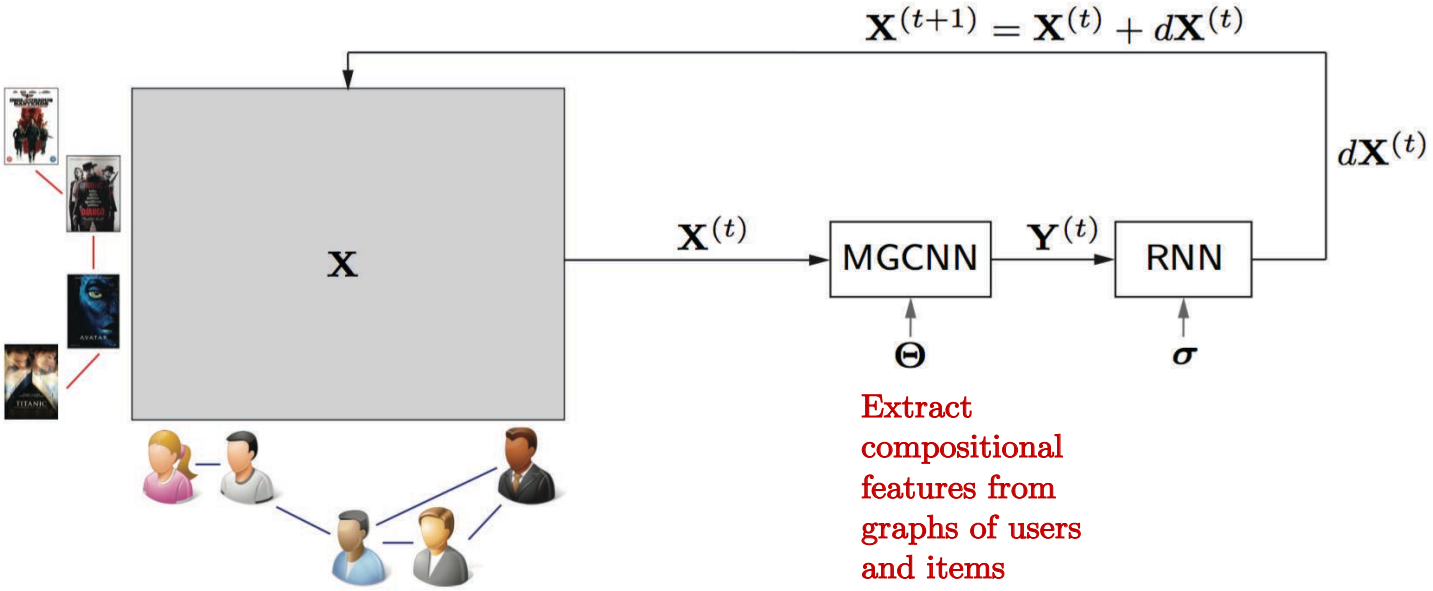
- Two spectral convolutional layers applied to each of the factors W, H

$$\mathbf{u}_l = \xi\left(\sum_{l'=1}^{p}\sum_{j=0}^{r}\theta_{\mathrm{r},jll'}T_j(\tilde{\mathbf{\Delta}}_{\mathrm{r}})\mathbf{w}_{l'}\right) \qquad \begin{array}{l} l=1,\dots,q \\ l'=1,\dots,p \end{array}$$

$$\mathbf{v}_l = \xi\left(\sum_{l'=1}^{p}\sum_{j'=0}^{r}\theta_{\mathrm{c},j'll'}T_{j'}(\tilde{\mathbf{\Delta}}_{\mathrm{c}})\mathbf{h}_{l'}\right)$$

- ☺ Filters have guaranteed r-hops support on both graphs
- ☺ O(1) parameters per layer
- ☺ O(n+m) computational complexity (assuming sparse graphs)
- ☹ May loose some coupling information

Matrix completion with Recurrent Multi-Graph ConvNets[25]



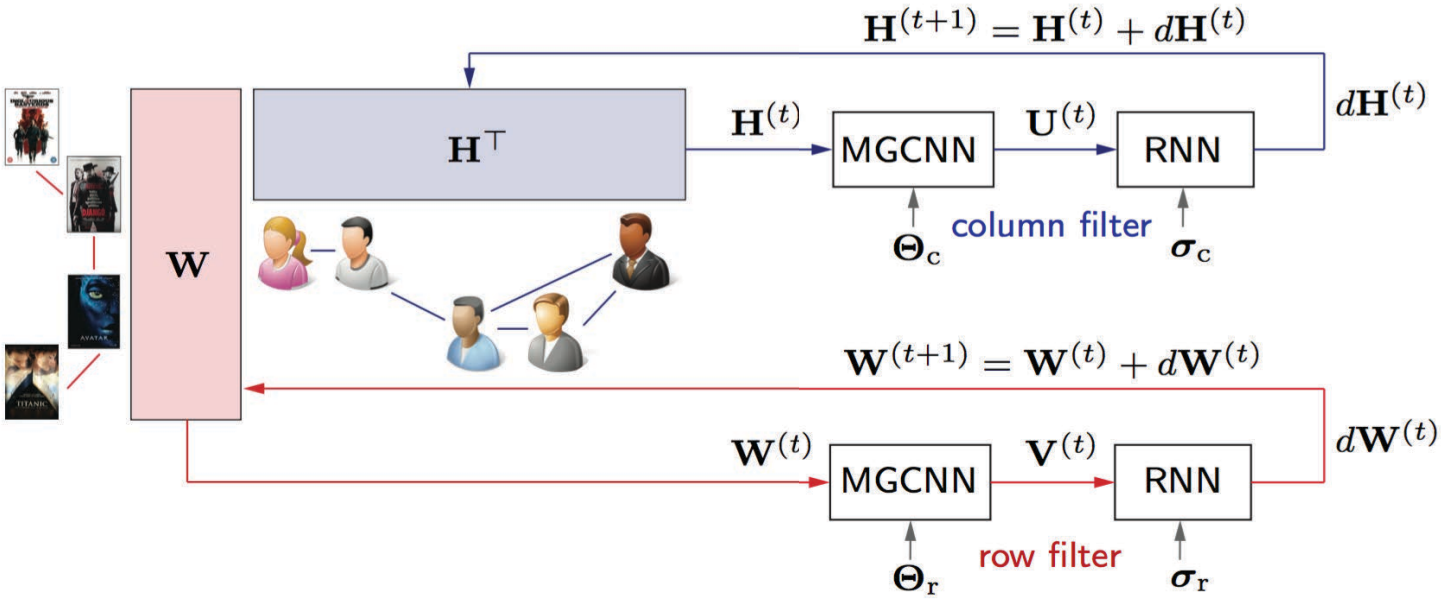
Recurrent multigraph CNN (RMCNN) architecture for matrix completion

$$\min_{\boldsymbol{\Theta},\boldsymbol{\sigma}} \|\mathbf{X}^{(T)}_{\boldsymbol{\Theta},\boldsymbol{\sigma}}\|^2_{\mathcal{G}_\mathrm{r}} + \|\mathbf{X}^{(T)}_{\boldsymbol{\Theta},\boldsymbol{\sigma}}\|^2_{\mathcal{G}_\mathrm{c}} + \frac{\mu}{2}\|\boldsymbol{\Omega} \circ (\mathbf{X}^{(T)}_{\boldsymbol{\Theta},\boldsymbol{\sigma}} - \mathbf{Y})\|^2_\mathrm{F}$$

Complexity: $\mathrm{O}(nm)$

[25] Monti, Bresson, Bronstein 2017

Factorized version



Separable recurrent multigraph CNN (sRMCNN) architecture
for matrix completion in factorized form

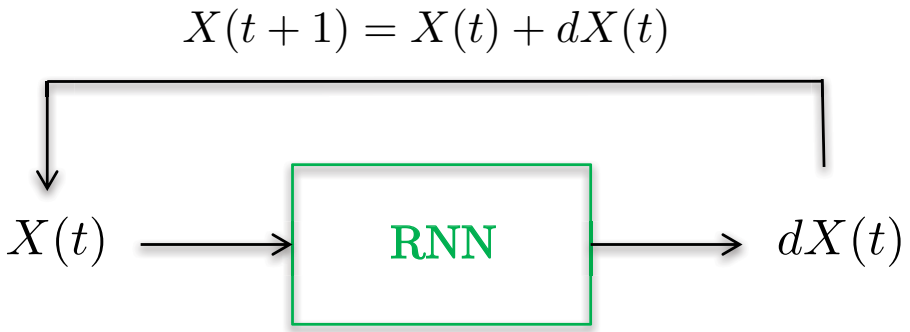
$$\min_{\boldsymbol{\theta}_\mathrm{r},\boldsymbol{\theta}_\mathrm{r},\boldsymbol{\sigma}_\mathrm{r},\boldsymbol{\sigma}_\mathrm{c}} \|\mathbf{W}^{(T)}_{\boldsymbol{\theta}_\mathrm{r},\boldsymbol{\sigma}_\mathrm{r}}\|^2_{\mathcal{G}_\mathrm{r}} + \|\mathbf{H}^{(T)}_{\boldsymbol{\theta}_\mathrm{c},\boldsymbol{\sigma}_\mathrm{c}}\|^2_{\mathcal{G}_\mathrm{c}} + \frac{\mu}{2}\|\mathbf{\Omega} \circ (\mathbf{W}^{(T)}_{\boldsymbol{\theta}_\mathrm{r},\boldsymbol{\sigma}_\mathrm{r}}(\mathbf{H}^{(T)}_{\boldsymbol{\theta}_\mathrm{c},\boldsymbol{\sigma}_\mathrm{c}})^\top - \mathbf{Y})\|^2_\mathrm{F}$$

Complexity: $\mathrm{O}(n+m)$

[25] Monti, Bresson, Bronstein 2017

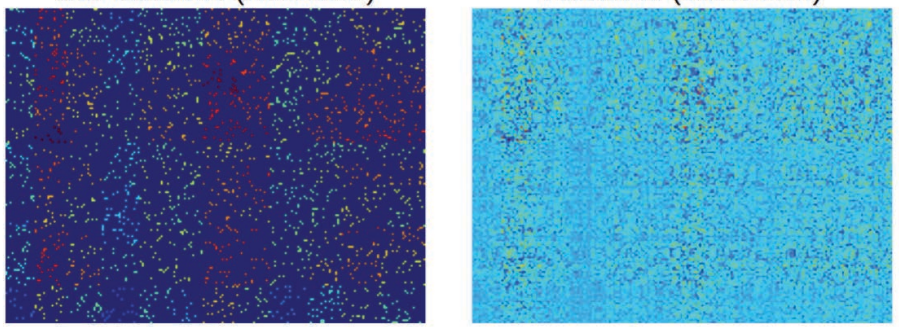
Incremental updates with RNNs

- The RNN/LSTM[26] cast the completion problem as non-linear diffusion process.
  - Replace multi-layer CNNs by simple RNN + diffusion
    ⇒ much less parameters to learn (reduce overfitting).
    ⇒ more favorable for highly sparse entries (better info diffusion).
  - Fix #parameters of the model independently of entry sparsity.
  - Allows to learn temporal dynamics of entries if such information is available.

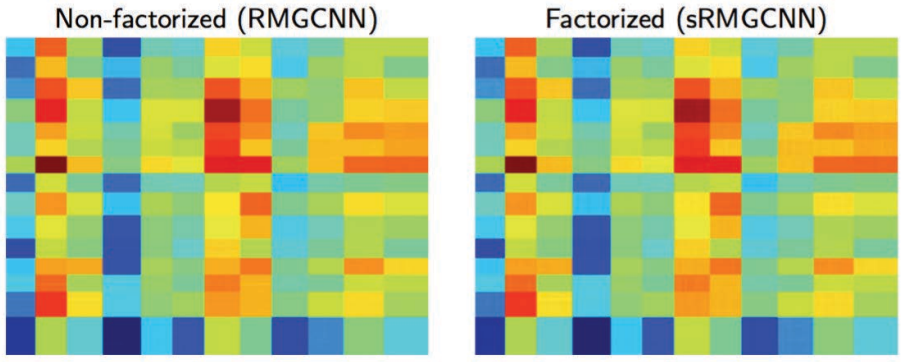


[26] Hochreiter, Schmidhuber 1997

Matrix completion methods comparison: synthetic



Matrix completion results on a synthetic dataset (initialization)



Matrix completion results on a synthetic dataset after $t = 10$ instances

Method	#Params	Complexity	RMSE
GMC[1]	mn	mn	0.3693
GRALS[2]	$m+n$	$m+n$	0.0114
sRMGCNN[3]	**1**	$\boldsymbol{m+n}$	**0.0106**
RMGCNN[3]	**1**	$\boldsymbol{mn}$	**0.0053**

Comparison of geometric matrix completion methods on synthetic data using both user+movie graphs

Methods: [1]Kalofolias et al. 2014; [2]Rao et al. 2015; [3]Monti, Bresson, Bronstein 2017

Matrix completion methods comparison: real

Method	MovieLens[1]	Flixster[2]	Douban[3]	Yahoo[4]
IMC[5]	1.653	–	–	–
GMC[6]	0.996	–	–	–
MC[7]	0.973	–	–	–
GRALS[8]	0.945	1.245	0.833	38.042
sRGCNN (Cheb)[9]	**0.929**	**0.926**	**0.801**	**22.415**
sRGCNN (Cayley)[10]	**0.922**	–	–	–

Accuracy (RMS error) of matrix completion methods on real data

Data: [1]Miller et al. 2003; [2]Jamali, Ester 2010; [3]Ma et al. 2011; [4]Dror et al. 2012
Methods: [5]Jain, Dhillon 2013; [6]Kalofolias et al. 2014; [7]Candès, Recht 2012; [8]Rao et al. 2015; [9]Monti, Bresson, Bronstein 2017; [10]Levie et al. 2017

Outline

- Convolutional Neural Networks
  - *Architecture*
  - *Non-Euclidean Data*
- Spectral Graph Theory
  - *Graphs and operators*
  - *Spectral decomposition*
  - *Fourier analysis*
  - *Convolution*
  - *Coarsening*
- Spectral ConvNets
  - *SplineNets*
  - *ChebNets*
  - *GraphConvNets*
- Spectral ConvNets on Multiple Graphs
  - *Recommender Systems*
- **Conclusion**

Conclusion

- Contributions:
  - Generalization of ConvNets to data on (fixed) graphs
  - Linear complexity for sparse graphs
  - GPU implementation
  - Multiple graphs
- Several potential applications in network sciences.

Questions?