Convolutional Neural Networks on Graphs

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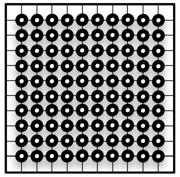
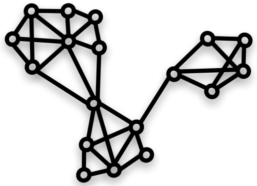
Outline

- **Part 1: Euclidean ConvNets**
  - *Architecture*
  - *Non-Euclidean data*

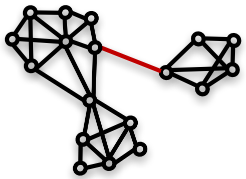


- **Part 2: Spectral ConvNets for Fixed Graphs**



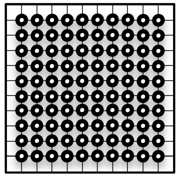
  - **Spectral Graph Theory**
    - *Graph convolution*
    - *Graph coarsening*
  - **Spectral ConvNets**
    - *SplineNets*
    - *ChebNets* [NIPS'16]*
    - *GraphConvNets*
    - *CayleyNets**
    - *Multiple fixed graphs* [NIPS'17]*

- **Part 3: ConvNets for Variable Graphs**
  - *Graph learning problems**

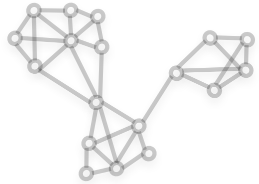


- **Conclusion**

Outline

➢ **Part 1: Euclidean ConvNets** 

- *Architecture*
- *Non-Euclidean data*

➢ Part 2: Spectral ConvNets for Fixed Graphs 

➢ Spectral Graph Theory

- *Graph convolution*
- *Graph coarsening*

➢ Spectral ConvNets

- *SplineNets*
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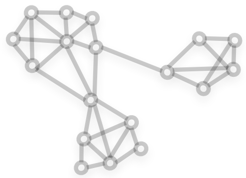
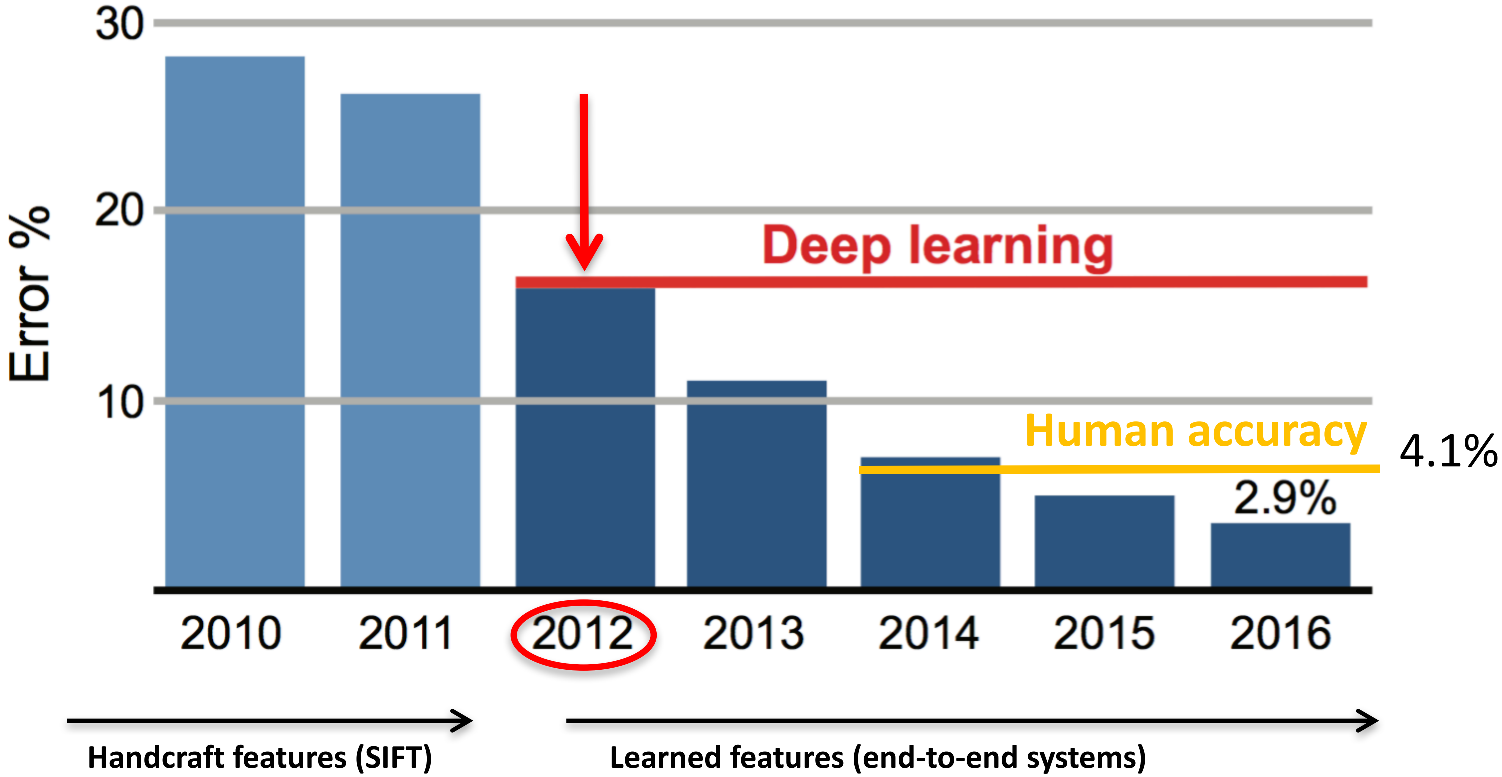
➢ Part 3: ConvNets for Variable Graphs 

- *Graph learning problems**

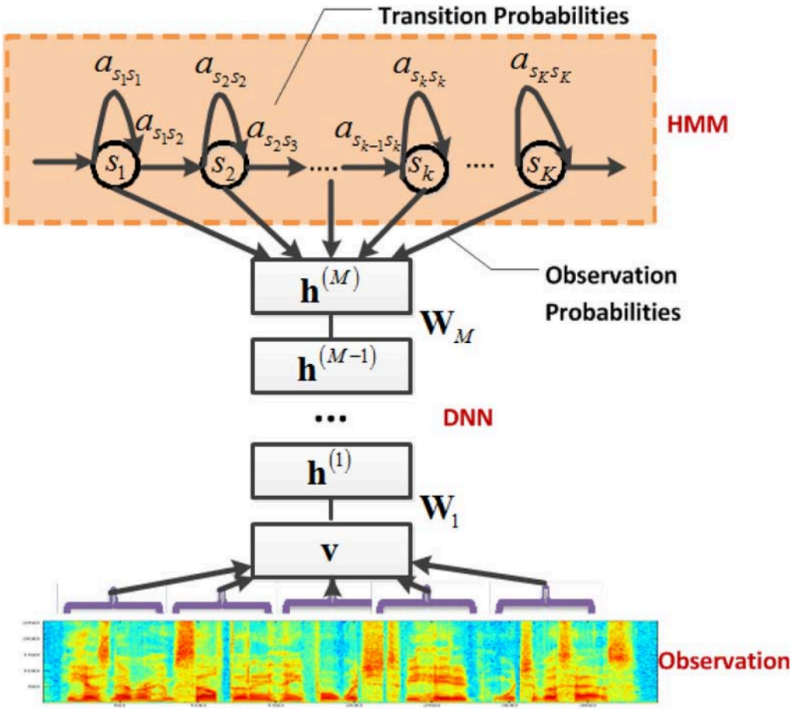
➢ Conclusion

ConvNets: A breakthrough in image recognition...



[1] LeCun, Bottou, Bengio, Haffner 1998
[2] Krizhevsky, Sutskever Hinton, 2012

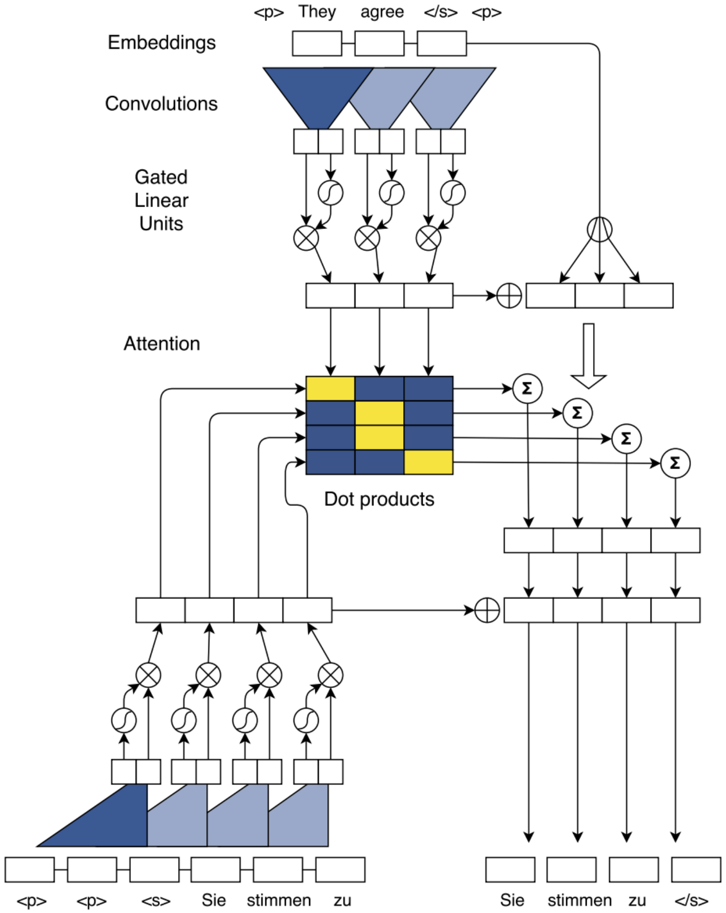
in speech recognition...



Acoustic model	Recog \ WER	RT03S FSH	Hub5 SWB
Traditional features	1-pass −adapt	27.4	23.6
Deep Learning	1-pass −adapt	18.5	16.1

[3] Dahl, Yu, Deng, Acero, 2010
[4] Hinton, Deng, Yu, Dahl et al. 2012

in language translation...



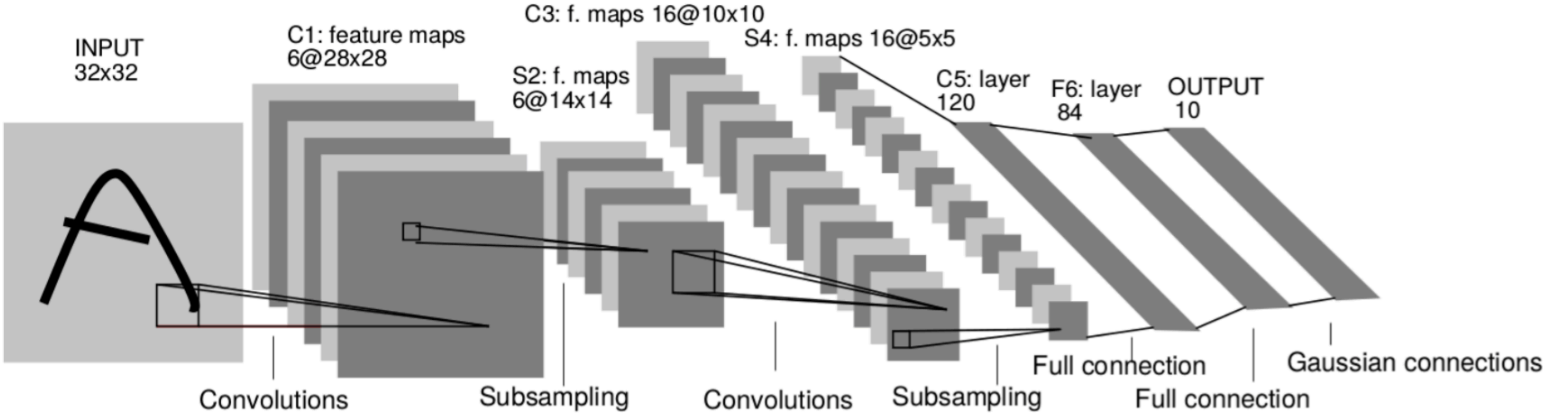
WMT'14 English-German	BLEU
Wu et al. (2016) GNMT	26.20
Wu et al. (2016) GNMT + RL	26.30
ConvS2S	26.43

WMT'14 English-French	BLEU
Zhou et al. (2016)	40.4
Wu et al. (2016) GNMT	40.35
Wu et al. (2016) GNMT + RL	41.16
ConvS2S	41.44
ConvS2S (10 models)	41.62

	BLEU	Time (s)
GNMT GPU (K80)	31.20	3,028
GNMT CPU 88 cores	31.20	1,322
GNMT TPU	31.21	384
ConvS2S GPU (K40) $b = 1$	33.45	327
ConvS2S GPU (M40) $b = 1$	33.45	221
ConvS2S GPU (GTX-1080ti) $b = 1$	33.45	142
ConvS2S CPU 48 cores $b = 1$	33.45	142
ConvS2S GPU (K40) $b = 5$	34.10	587
ConvS2S CPU 48 cores $b = 5$	34.10	482
ConvS2S GPU (M40) $b = 5$	34.10	406
ConvS2S GPU (GTX-1080ti) $b = 5$	34.10	256

[5] Gehring, Auli, Grangier, Yarats, Dauphin, 2017

An architecture for high-dimensional learning

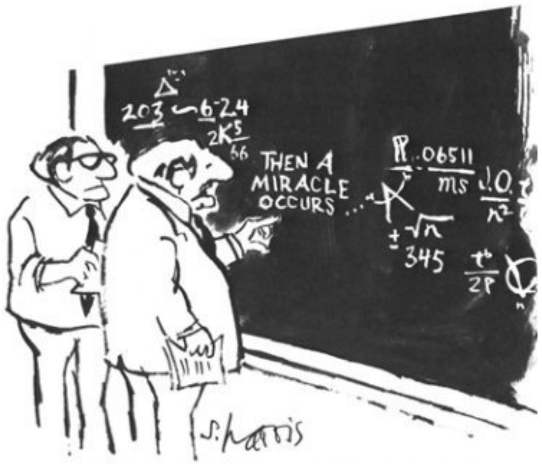


- **Curse of dimensionality:**

  dim(image) = 512 x 512 ≈ 10^6

  For N=10 samples/dim ⇒ $10^{1,000,000}$ points

- **ConvNets are powerful to solve high-dimensional learning problems.**

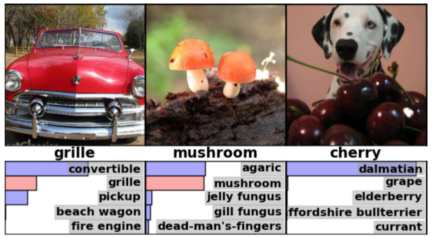


"I think you should be more explicit here in step two."

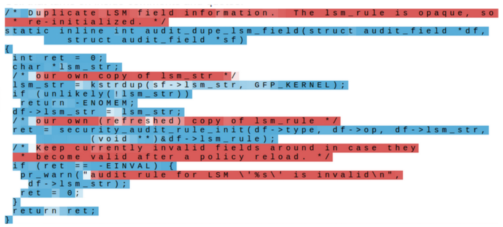
ConvNets

- Main assumption: Data (images, videos, sounds) are compositional, they are formed of patterns that are:
  - Local
  - Stationary
  - Multi-scale (hierarchical)

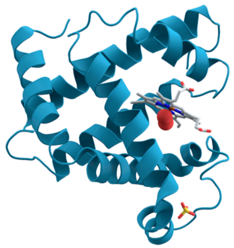
- ConvNets leverage the compositionality structure: They extract compositional features and feed them to classifier, recommender, etc (end-to-end).



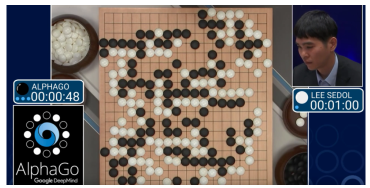
Computer Vision



NLP



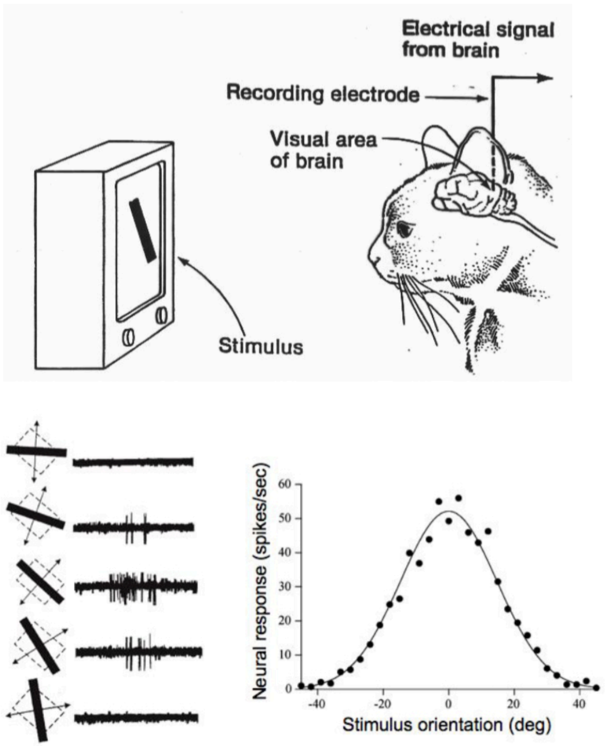
Drug discovery

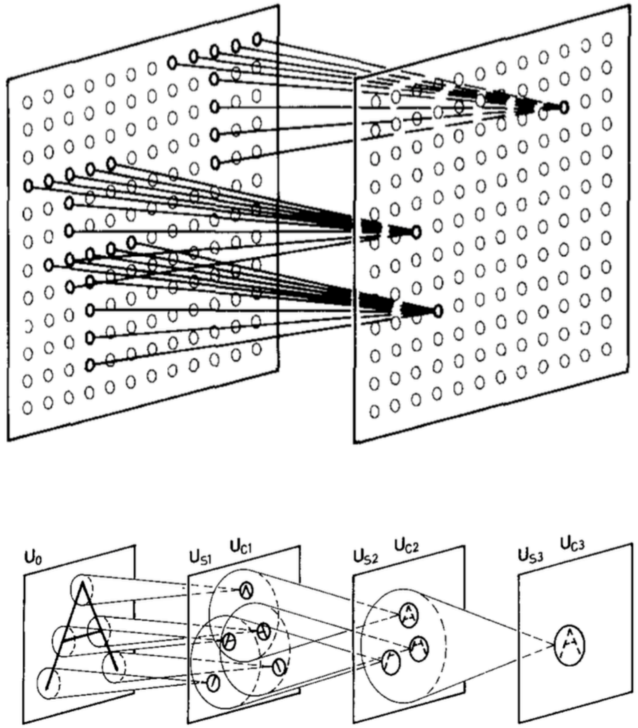


Games

Key property

- **Locality:** Property inspired by visual cortex neurons.
- **Local receptive fields**[6] activate in the presence of local features.





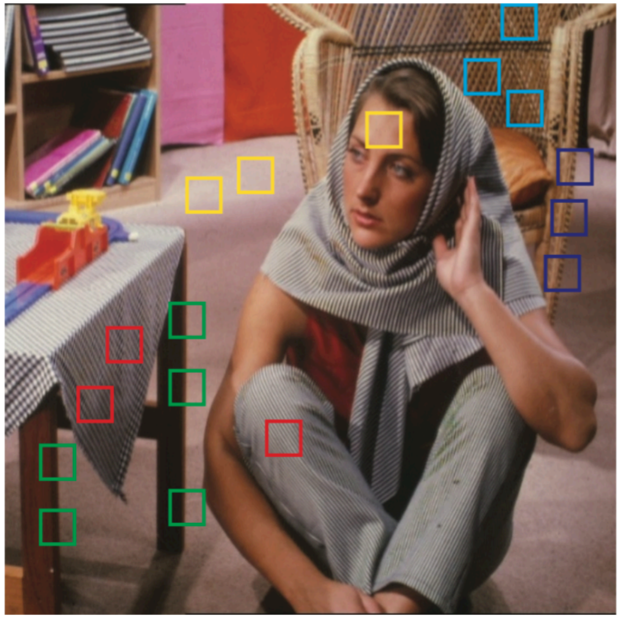
Neocognitron[7]

[6] Hubel, Wiesel 1962
[7] Fukushima 1980

Key property

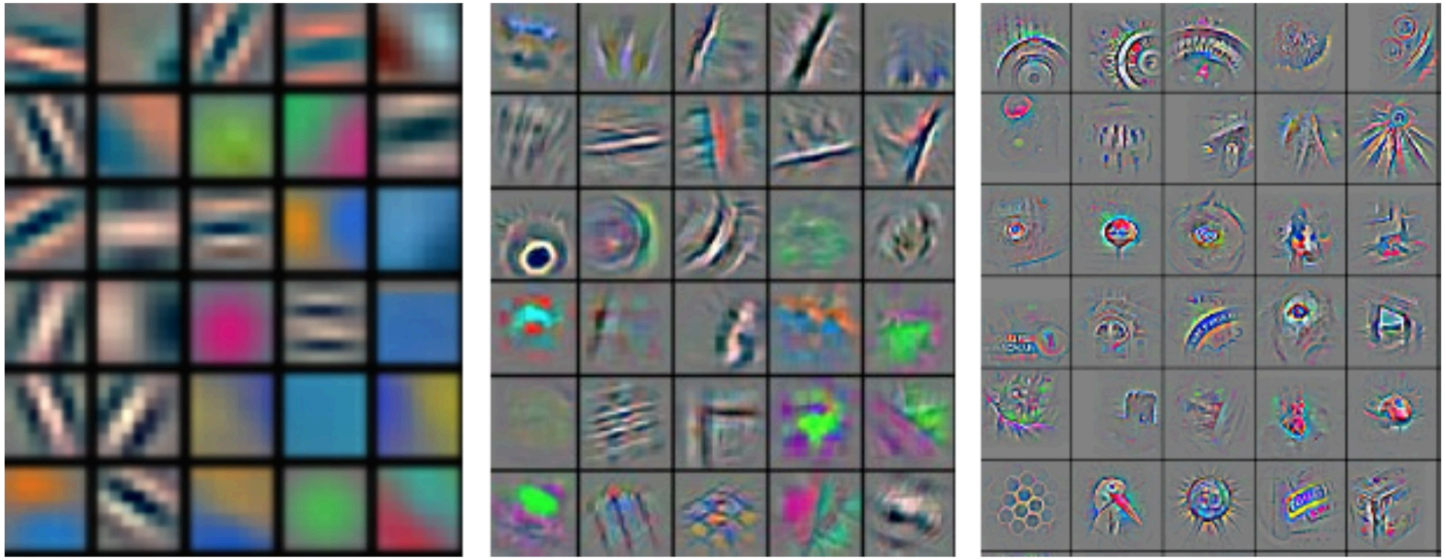
- Stationarity ⇔ Translation invariance (global invariance)

- Local stationarity ⇔ Similar patches are shared across the data domain (local invariance, good for intra-class variations)



Key property

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

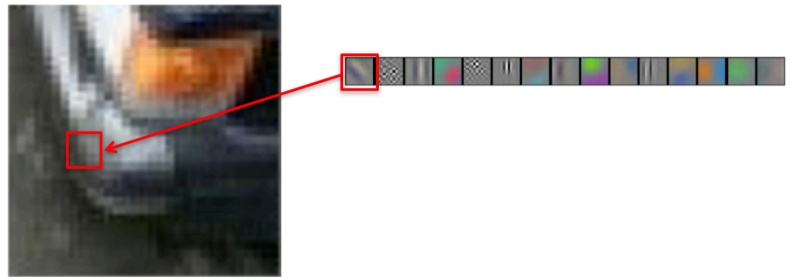


Features learned by ConvNet become increasingly more complex at deeper layers[8].

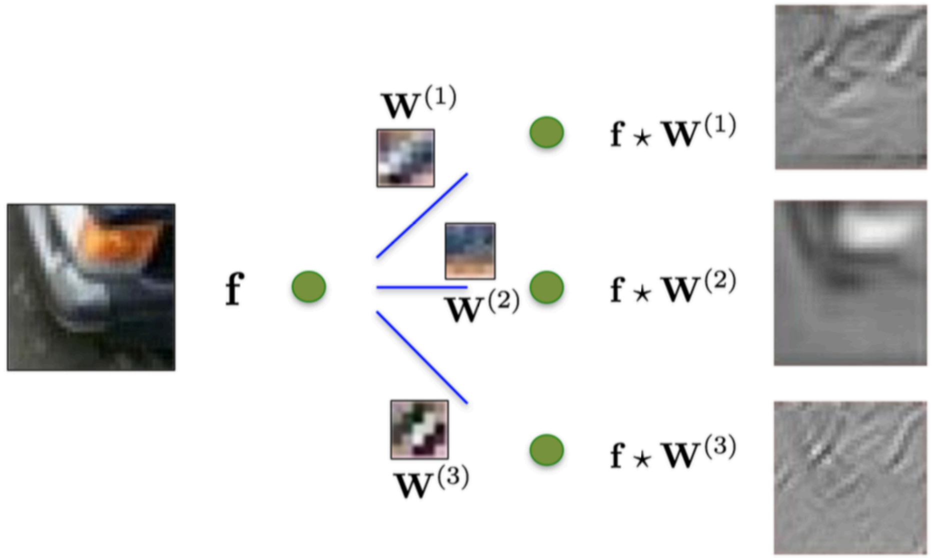
[8] Zeiler, Fergus 2013

Implementation complexity

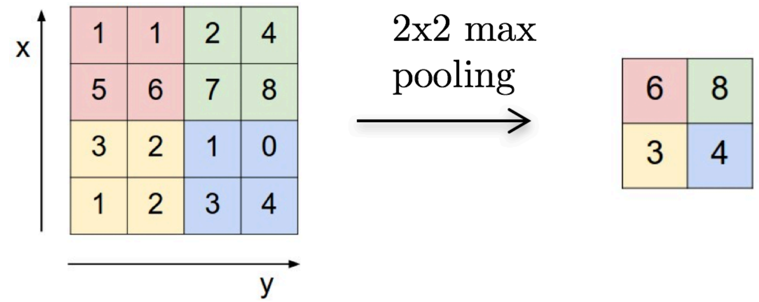
- **Locality:** Compact support kernels $\Rightarrow O(1)$ parameters per filter.



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

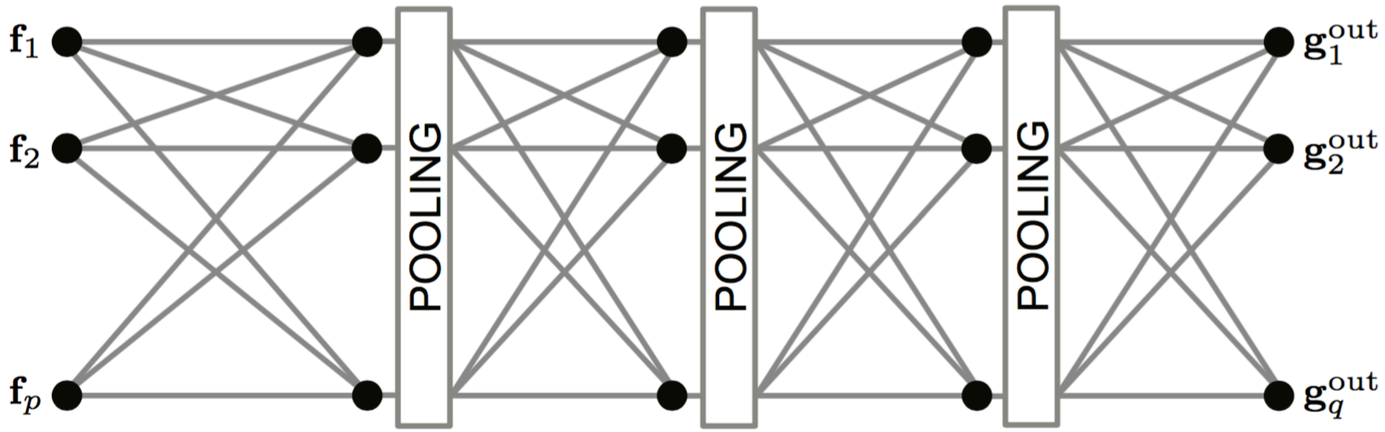


- **Multi-scale:** Downsampling + pooling $\Rightarrow O(n)$



Compositional layers

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



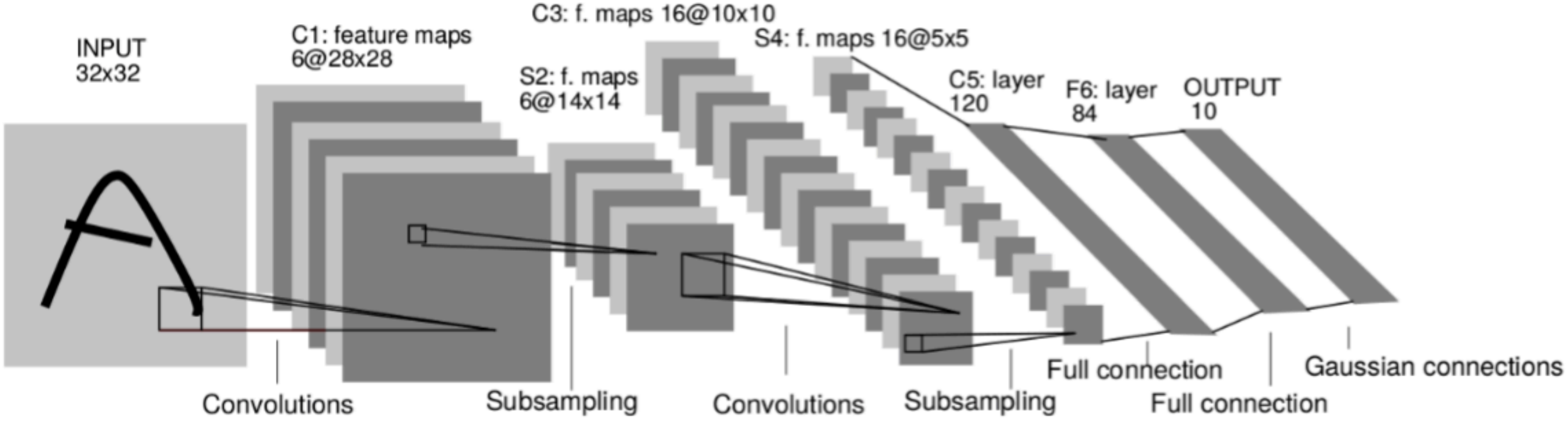
Compositional features consist of multiple convolutional + pooling layers.

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

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

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

ConvNets



- ☺ 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)

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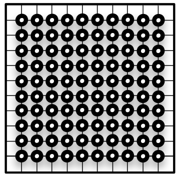
- **Part 1: Euclidean ConvNets** 
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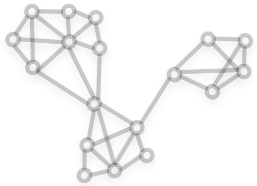

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  - Spectral Graph Theory
    - *Graph convolution*
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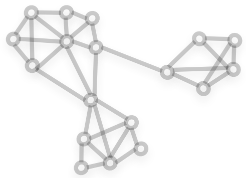
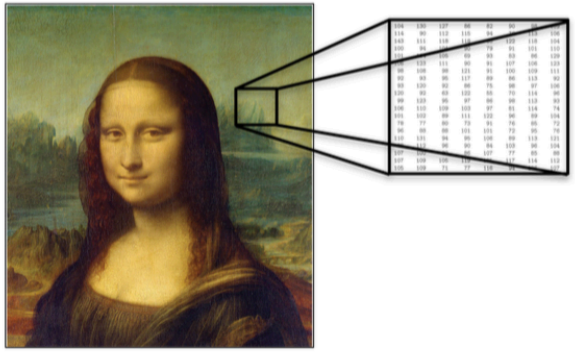


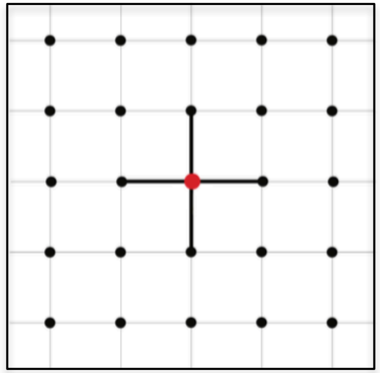
- Part 3: ConvNets for Variable Graphs
  - *Graph learning problems**

- Conclusion

Data domain for ConvNets

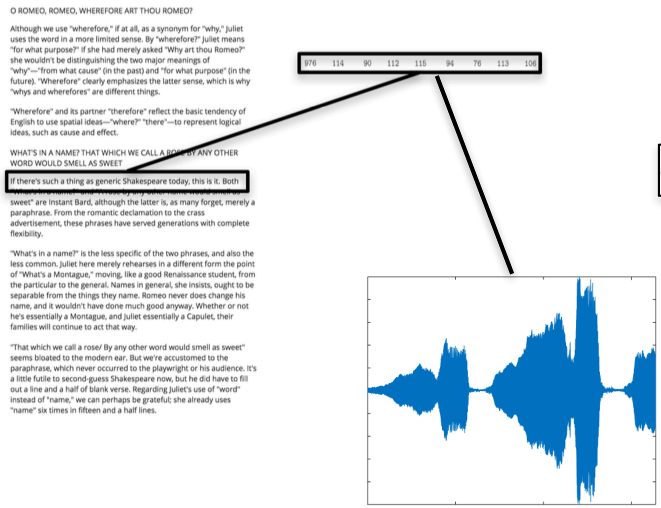
- Image, volume, video: 2D, 3D, 2D+1 Euclidean domains

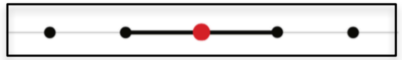




2D grids

- Sentence, word, sound: 1D Euclidean domain



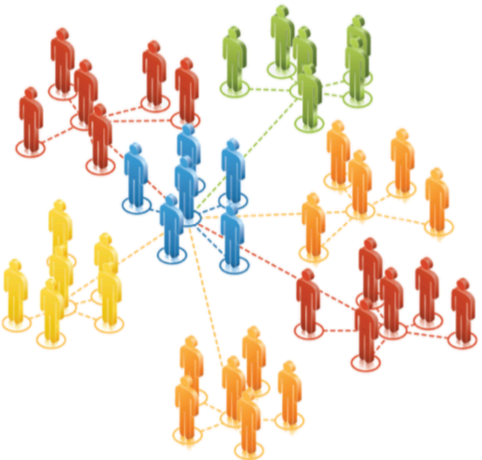


1D grid

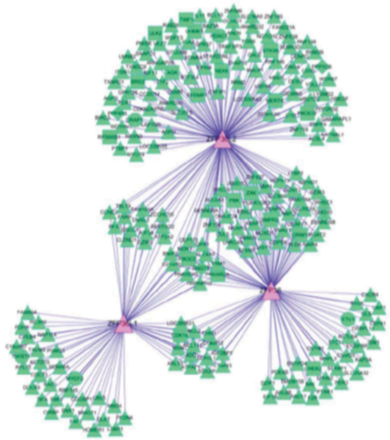
- These domains have nice regular spatial structures.

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

Non-Euclidean data

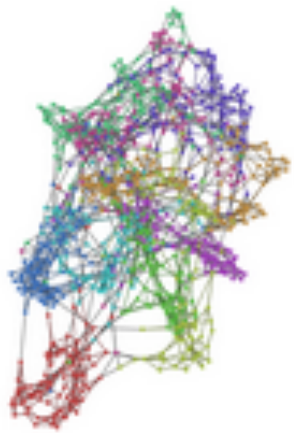


Social networks

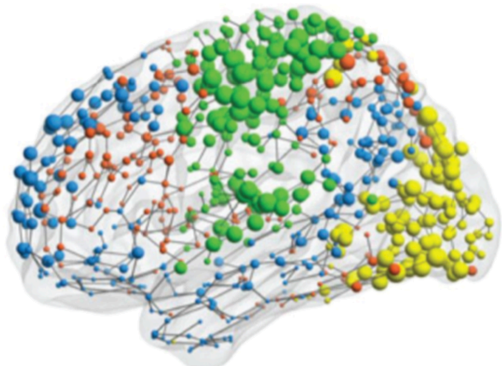


Regulatory networks

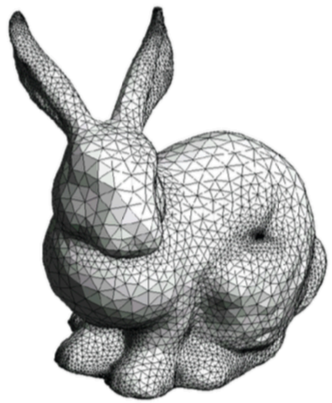
=



Graphs/
Networks



Functional networks



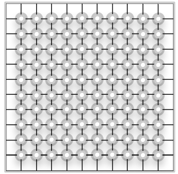
3D shapes

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

Challenges

- How to extend ConvNets 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)

Outline



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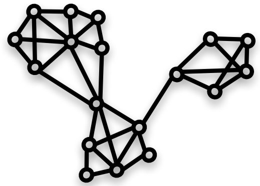

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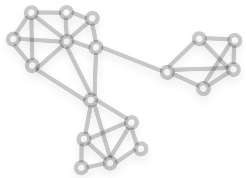
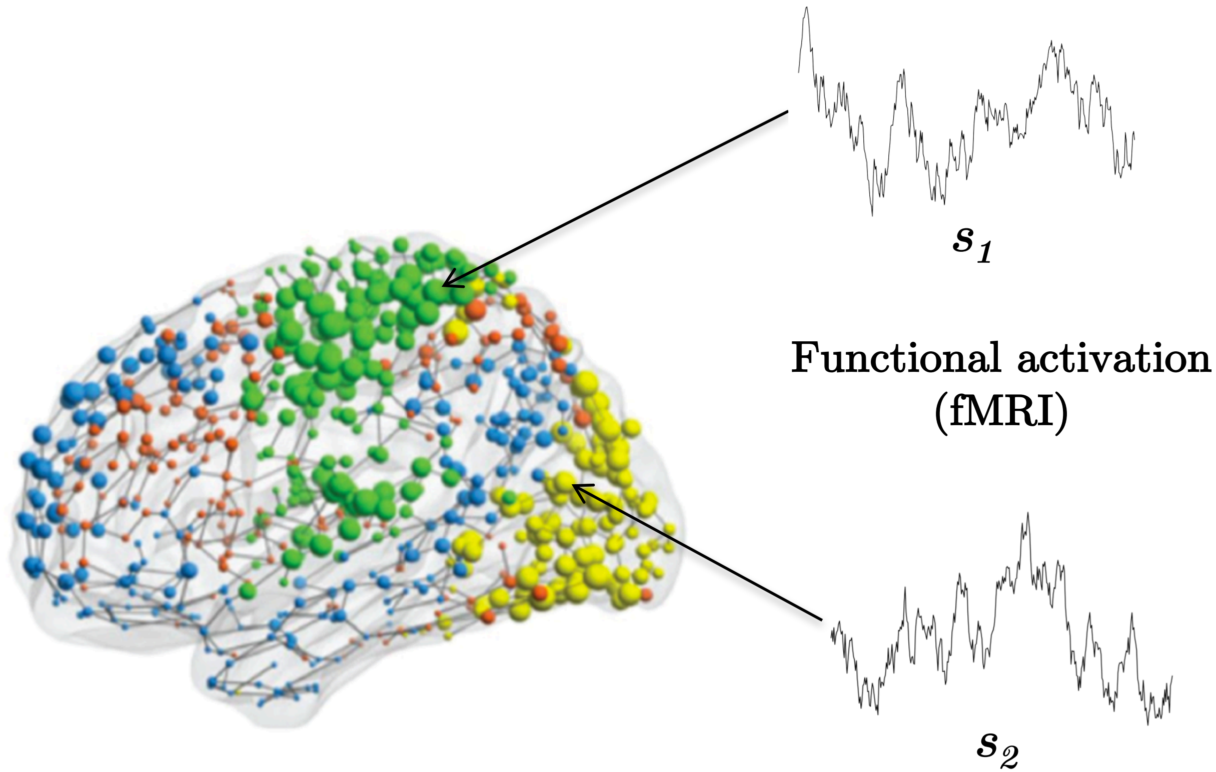


- Part 3: ConvNets for Variable Graphs
  - *Graph learning problems**

- Conclusion

Problem setting

- Given fixed graph(s) G, and a set of signals s_k on G to be analyzed with ConvNets:

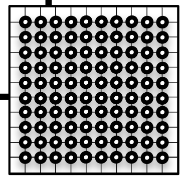


Brain connectivity network (sMRI)
Fixed graph G

Spectral ConvNets

Signal s_k: Image

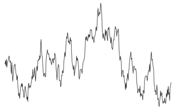
Part 1:
(Euclidean)
ConvNets



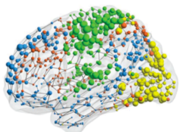
Classification

New data domain

Signal s_k: fMRI



Part 2:
Non-Euclidean
ConvNets



Fixed graph G

Classification

What do we need to generalize?

- Convolution and downsampling must be generalized from Euclidean grid domains to graphs. How?

  - Spectral graph theory allows to redefine convolution in the context of graphs with Fourier analysis.

  - Graph theory provide graph clustering techniques to reformulate downsampling for graphs.

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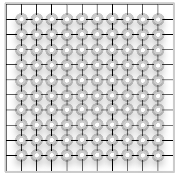

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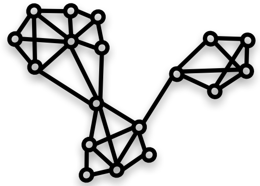

  - **Spectral Graph Theory**
    - *Graph convolution: Graphs, Fourier modes, Fourier analysis, convolution*
    - *Graph coarsening: Graph clustering, HEM, binary tree indexing*
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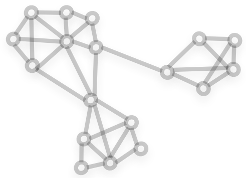


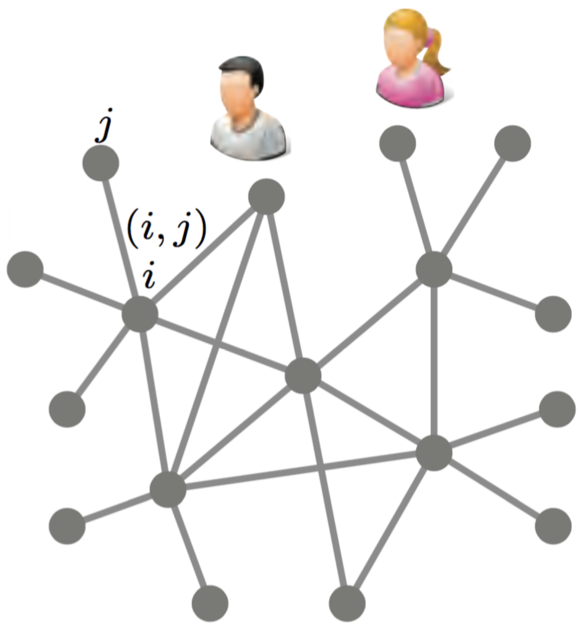
- Conclusion

Graphs

- **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** $L^2(\mathcal{V}) = \{f : \mathcal{V} \to \mathbb{R}^h\}$

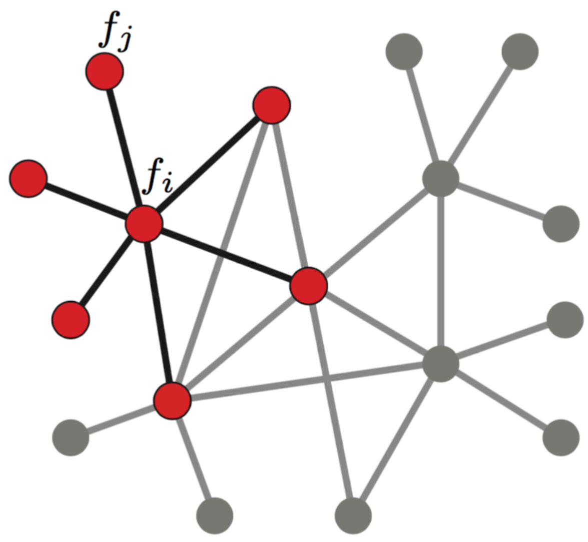
  Represented as $\mathbf{f} = (f_1, \ldots, f_n)$
- **Hilbert space with inner product**

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



[9] 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 (2$^{\text{nd}}$ derivative on graphs)

- Core operator in spectral graph theory.

- Represented as a positive semi-definite $n \times n$ matrix
  - Unnormalized Laplacian $\quad \boldsymbol{\Delta} = \mathbf{D} - \mathbf{A}$
  - Normalized Laplacian $\quad \boldsymbol{\Delta} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$
  - Random walk Laplacian $\quad \boldsymbol{\Delta} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{A}$

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

Outline

- Part 1: Euclidean ConvNets
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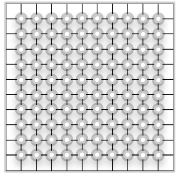
  - *Non-Euclidean data*



- **Part 2: Spectral ConvNets for Fixed Graphs**
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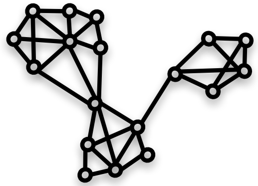
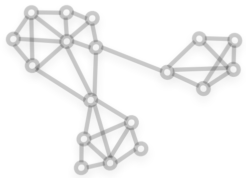


- Part 3: ConvNets for Variable Graphs
  - *Graph learning problems**



- Conclusion

Spectral decomposition

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

$$\mathbf{\Delta}\phi_k = \lambda_k \phi_k, \qquad k = 1, 2, \ldots$$

  - Eigenvectors are real and orthonormal (self-adjointness) $\langle \phi_k, \phi_{k'} \rangle_{L^2(\mathcal{V})} = \delta_{kk'}$
  - Eigenvalues are non-negative (positive-semidefiniteness) $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$
  - Laplacian eignenvectors are also called Fourier basis functions/modes.

- Eigendecomposition of graph Laplacian:

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

where $\mathbf{\Phi} = (\phi_1, \ldots, \phi_n)$ and $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$

Interpretation

- Find the smoothest orthonormal basis $\boldsymbol{\Phi} = (\phi_1, \ldots, \phi_n)$ on a graph

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

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

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

- Solution: first n Laplacian eigenvectors

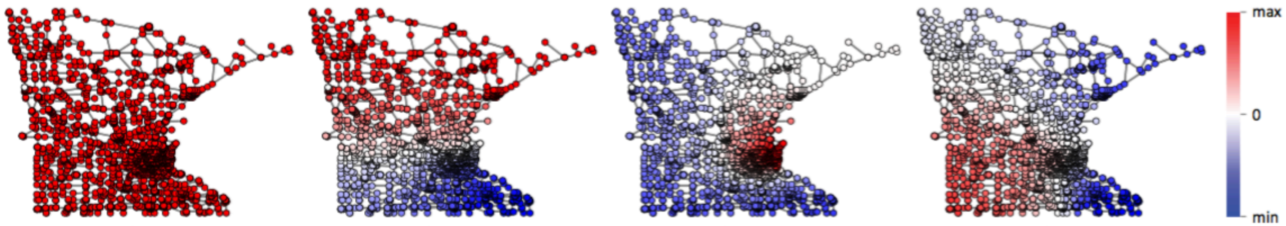
$$\min_{\boldsymbol{\Phi} \in \mathbb{R}^{n \times n}} \underbrace{\mathrm{trace}(\boldsymbol{\Phi}^\top \boldsymbol{\Delta} \boldsymbol{\Phi})}_{\|\boldsymbol{\Phi}\|_{\mathcal{G}} \text{ Dirichlet norm}} \quad \text{s.t.} \quad \boldsymbol{\Phi}^\top \boldsymbol{\Phi} = \mathbf{I}$$

Fourier modes

- Euclidean domain:

First eigenvectors of 1D Euclidean Laplacian = standard Fourier basis

- Graph domain:



ϕ_0 ϕ_1 ϕ_2 ϕ_3

First Laplacian eigenvectors of a graph

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

[10] Von Luxburg 2007

Outline

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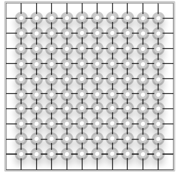

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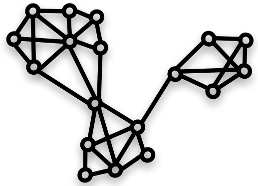

➢ **Spectral Graph Theory**

- *Graph convolution: Graphs, Fourier modes, Fourier analysis, convolution*
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➢ Spectral ConvNets

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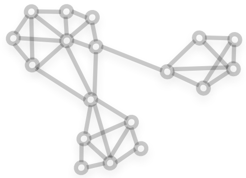


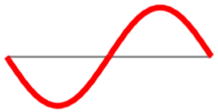
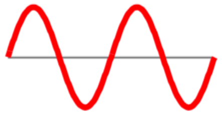
- *Graph learning problems**

➢ Conclusion

Euclidean Fourier analysis

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

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

f  $= \hat{f}_1$  $+ \hat{f}_2$  $+ \hat{f}_3$  $+ \ldots$

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

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

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

Fourier analysis on graphs

- A function $f : \mathcal{V} \to \mathbb{R}$ can be written as Fourier series[11]:

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

- $\hat{f}_k$ is the k-th graph Fourier coefficient.

- In matrix-vector notation, with the n x n Fourier matrix $\mathbf{\Phi} = [\phi_1, ..., \phi_n]$

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

Fourier transform

Inverse Fourier transform

- Graph Fourier basis ϕ_k = Laplacian eigenvectors :

$$\mathbf{\Delta}\phi_k = \lambda_k \phi_k \quad \text{with} \quad \begin{cases} \phi_k & = & \text{graph Fourier mode} \\ \lambda_k & = & \text{(square) frequency} \end{cases}$$

[11] Hammond, Vandergheynst, Gribonval, 2011

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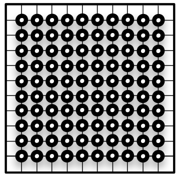

  - *Architecture*
  - *Non-Euclidean data*

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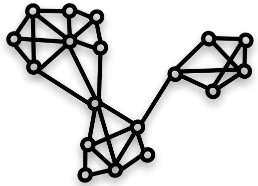

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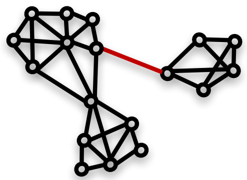


  - *Graph learning problems**

- Conclusion

Convolution in Euclidean space

- 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 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 in discrete Euclidean space

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

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

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

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

Convolution on graphs

- Spectral convolution of $f, g \in L^2(\mathcal{V})$ can be defined by analogy[11]

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

- In matrix-vector notation

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

  - Not shift-invariant (G has no circulant structure)
  - Filter coefficients depend on basis $\phi_1, \ldots, \phi_n$
  - Expensive computation (no FFT): $O(n^2)$

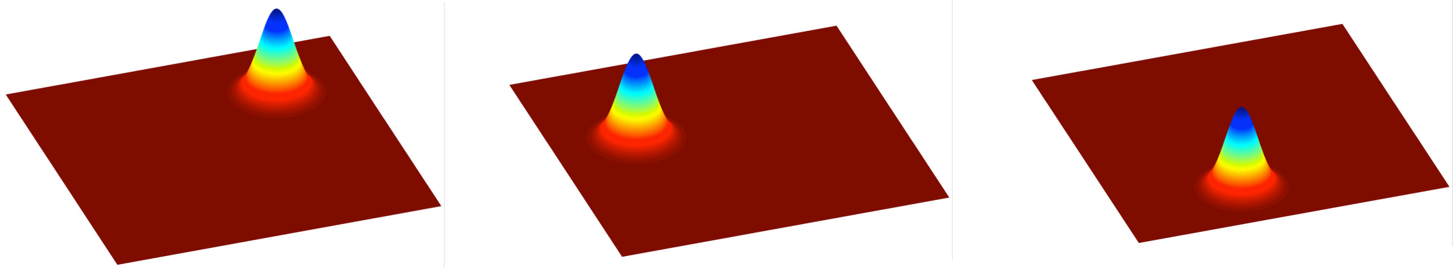
[11] Hammond, Vandergheynst, Gribonval, 2011

No shift invariance on graphs

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

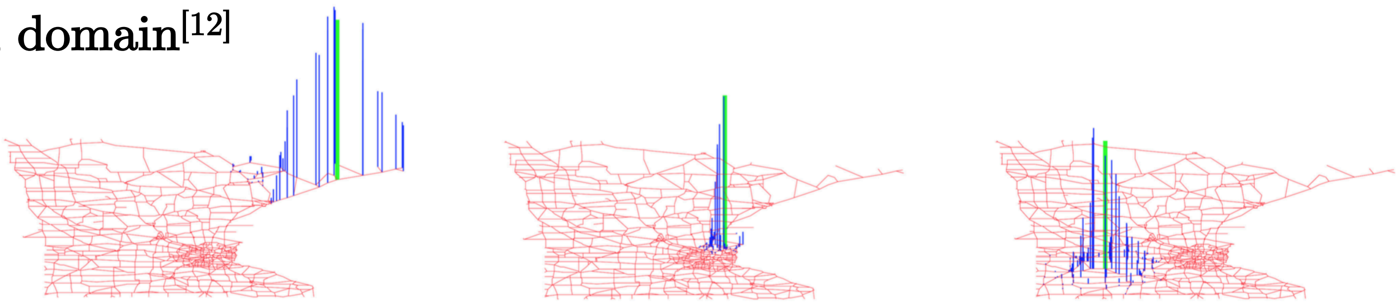
$$T_i \mathbf{f} = \mathbf{f} \star \boldsymbol{\delta}_i$$

- 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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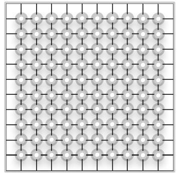

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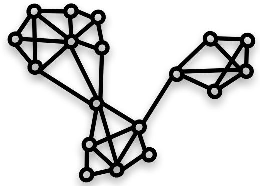

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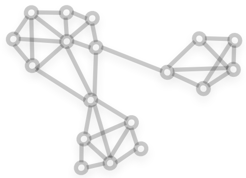


- Conclusion

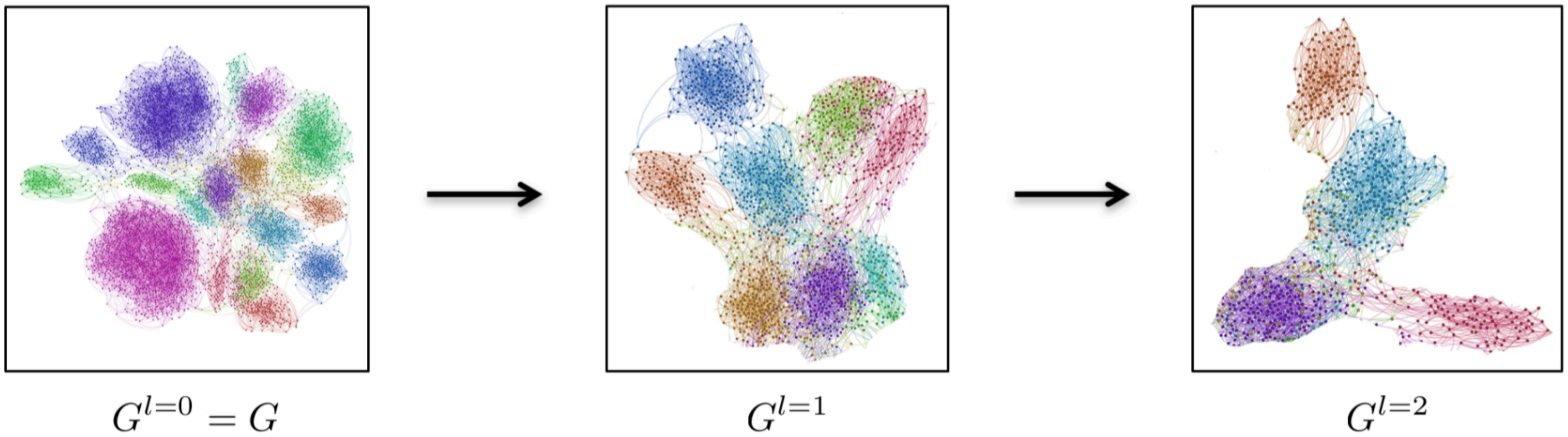
Graph dowsampling

- Goals:
  - Pool similar local features (max/average 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 dowsampling

- Graph downsampling $\Leftrightarrow$ graph coarsening $\Leftrightarrow$ graph partitioning: Decompose G into smaller meaningful clusters.



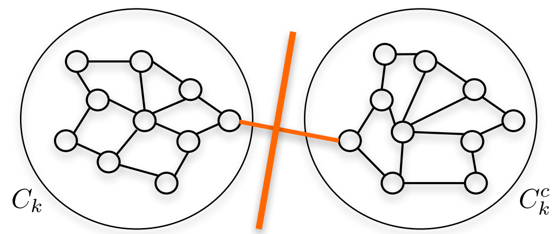
- Graph partitioning is NP-hard $\Rightarrow$ Approximation

Balanced cuts

- Powerful combinatorial graph partitioning models:

  - Normalized cut[13]

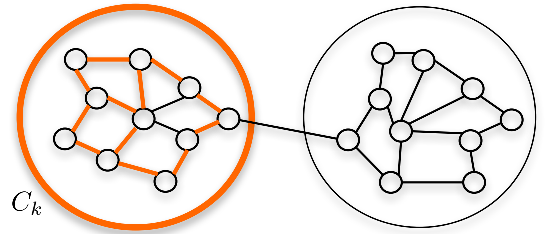
$$\min_{C_1,\ldots,C_K} \sum_{k=1}^{K} \frac{\mathrm{Cut}(C_k, C_k^c)}{\mathrm{Vol}(C_k)}$$



Partitioning by min edge cuts.

  - Normalized association

$$\max_{C_1,\ldots,C_K} \sum_{k=1}^{K} \frac{\mathrm{Assoc}(C_k)}{\mathrm{Vol}(C_k)}$$



Partitioning by max vertex matching.

where $\mathrm{Cut}(A,B) := \sum_{i\in A, j\in B} a_{ij}$, $\mathrm{Assoc}(A) := \sum_{i\in A, i\in B} a_{ij}$, $\mathrm{Vol}(A) := \sum_{i\in A, j\in B} d_i$, and $d_i := \sum_{j\in V} a_{ij}$.

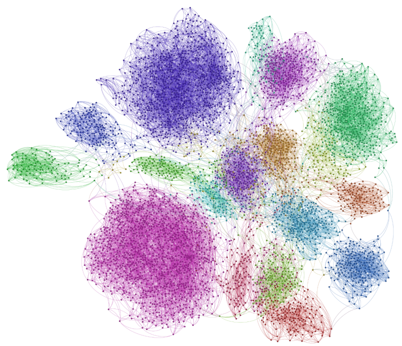
- Both models are equivalent, but lead to different algorithms.

[13] Shi, Malik, 2000

Balanced cuts

- Balanced cuts are NP-hard ⇒ most popular approximation techniques focus on linear spectral relaxation (eigenproblem with global solution).

- Graph geometry are generally not linear ⇒ Graclus[14] algorithm computes non-linear clusters that locally maximize the Normalized Association.



- Graclus algorithm offers a control of the coarsening ratio of ≈ 2 (like image grid) using heavy-edge matching[15].

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

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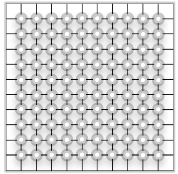

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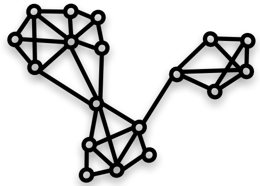

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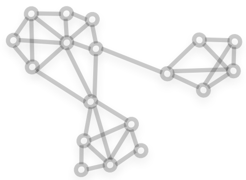
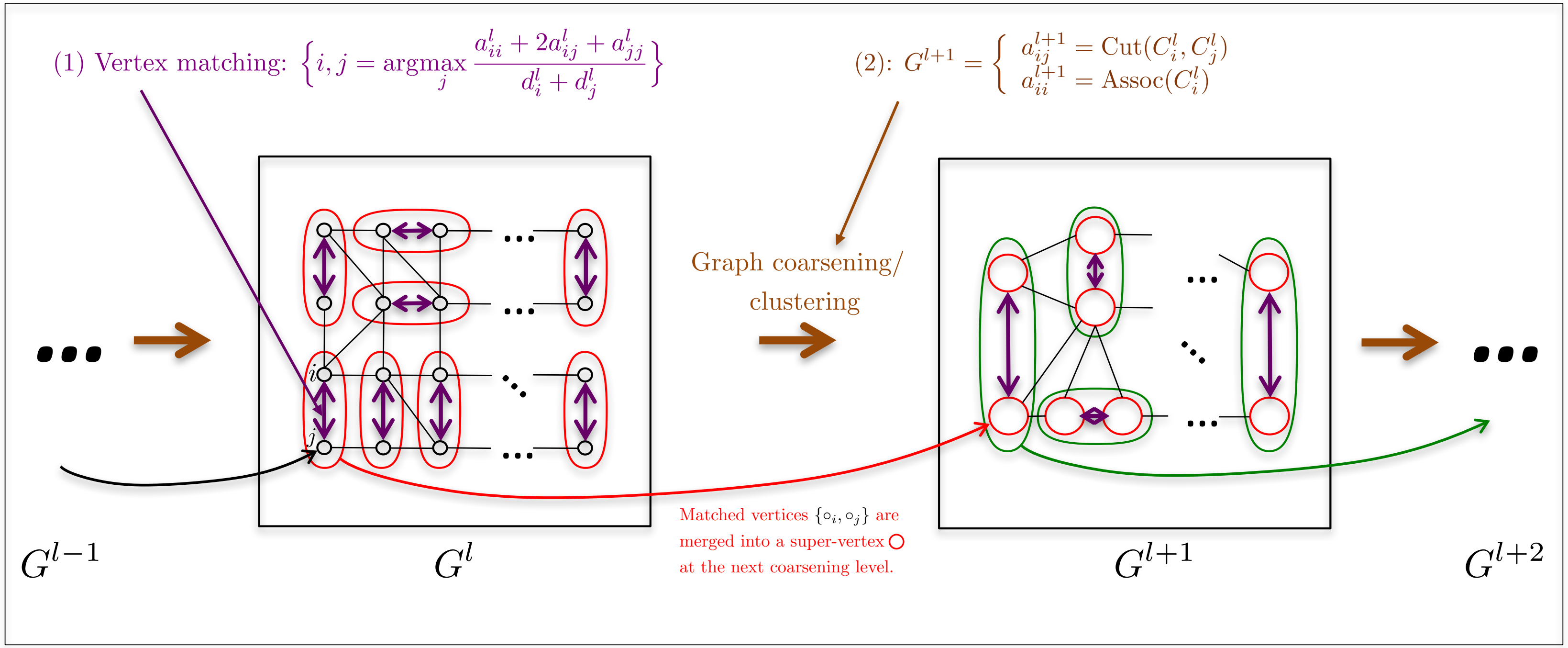


  - *Graph learning problems**

- Conclusion

Heavy-Edge Matching (HEM)

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



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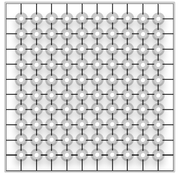

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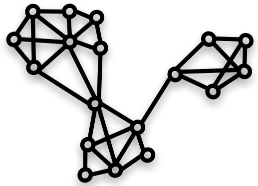

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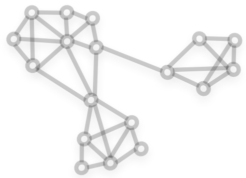
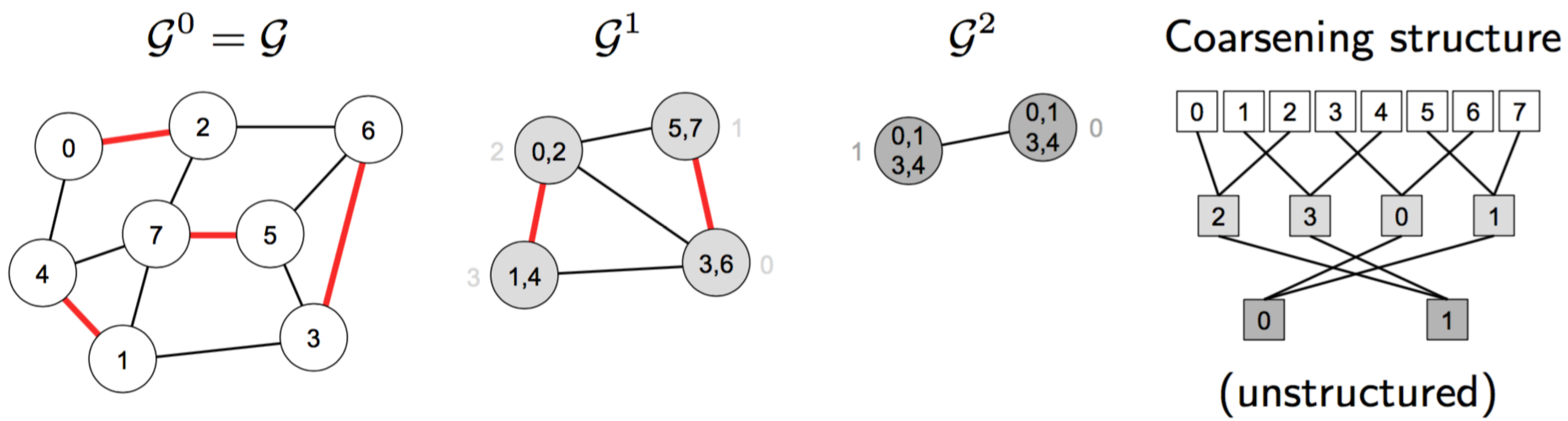


- Conclusion

Unstructured pooling

- Sequence of coarsened graphs produced by HEM:

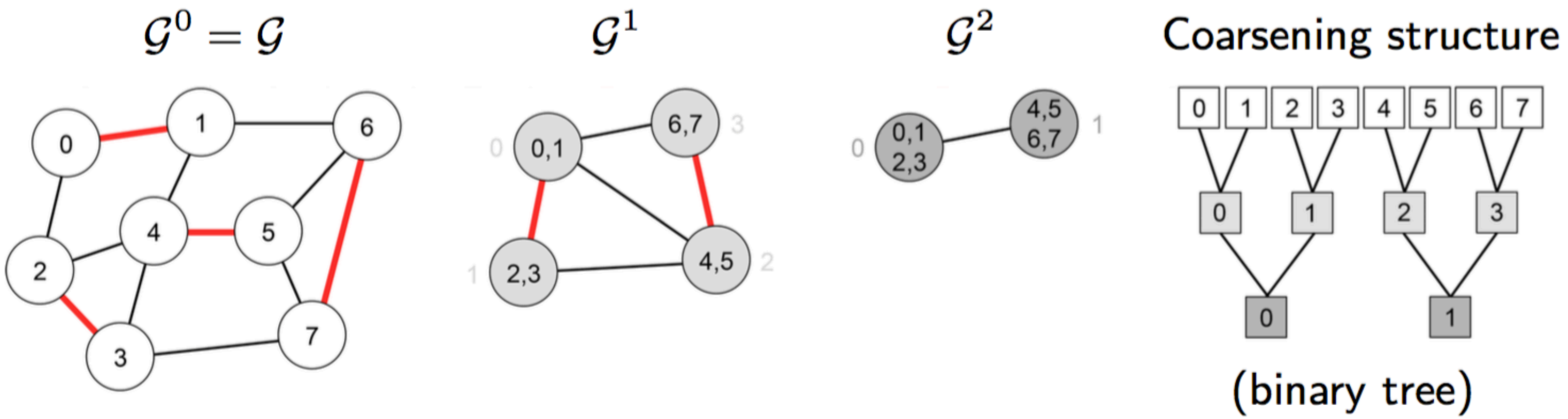


☹ Stores a table of indices for graph and all its coarsened versions

☹ Computationally inefficient

Fast graph pooling

- Structured pooling[18]: 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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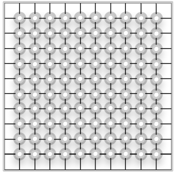

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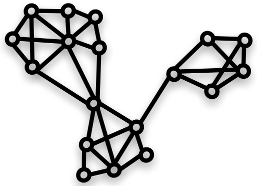

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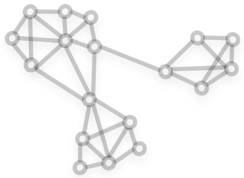
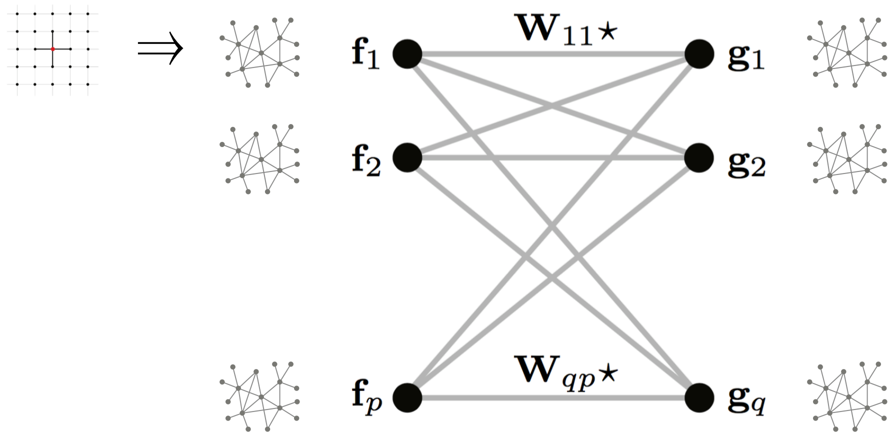


- Conclusion

Vanilla spectral graph ConvNets

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

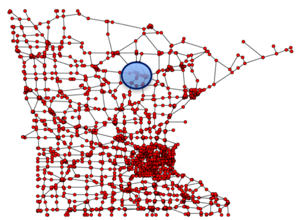
Activation, e.g. $\quad \xi(x) = \max\{x, 0\}$ $\quad$ rectified linear unit (ReLU)

[16] Bruna, Zaremba, Szlam, LeCun 2014

Spectral graph convolution

- Convolutional layer in the spatial domain:

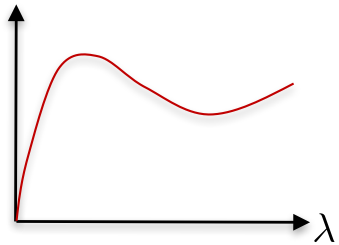
$$\mathbf{g}_l = \xi\left(\sum_{l'=1}^{p} \mathbf{W}_{l,l'} \star \mathbf{f}_{l'}\right),$$



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

- 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

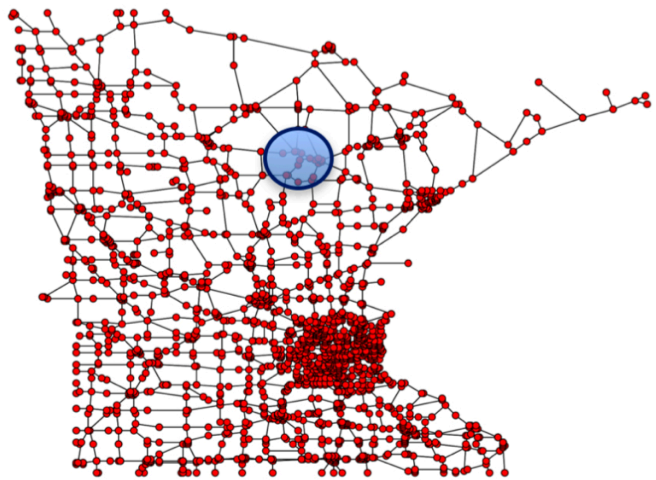
Spatial localization and spectral smoothness[17]

- **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**

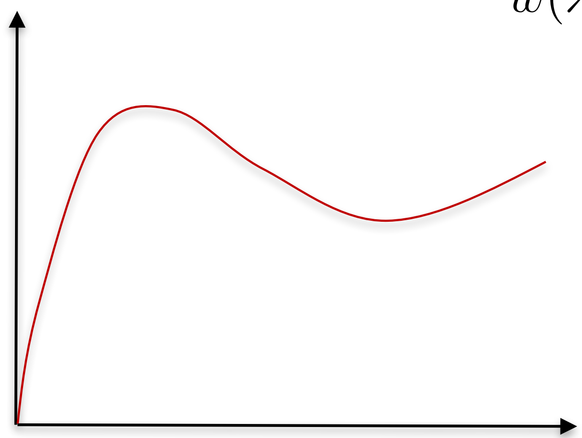
$w(x)$



Spatial localization

$\Leftrightarrow$

$\hat{w}(\lambda)$



λ

Smooth spectral filter function

[17] Henaff, Bruna, LeCun 2015

Smooth parametric spectral filter

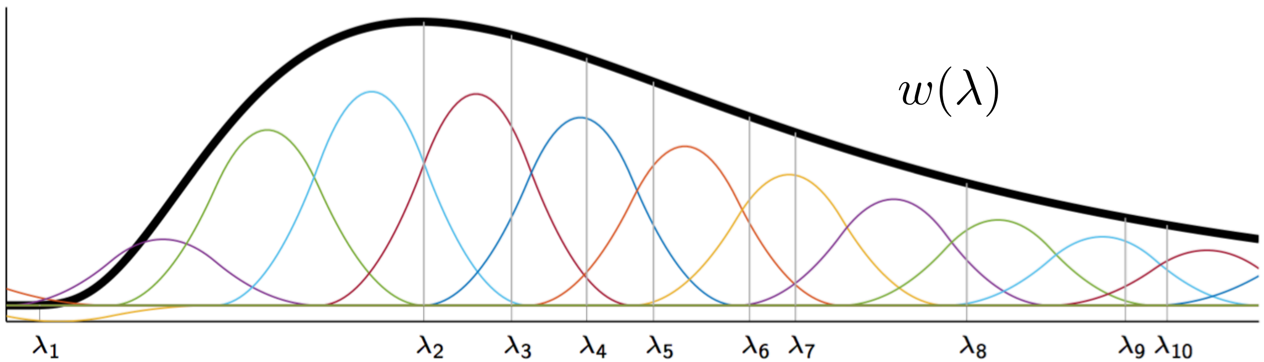
- **Parametrize the smooth spectral filter function** $w_(\lambda)$ **with a linear combination of smooth kernel functions** $\beta_1(\lambda), \ldots, \beta_r(\lambda)$ **, e.g. splines:**

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

$$\Downarrow$$

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

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



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

SplineNets

- Series of parametric spectral convolutional layers:

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

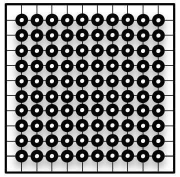
with smooth spectral parametric coefficients $\mathbf{W}_{l,l'}^{(k)}$ to be learned at each layer.

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

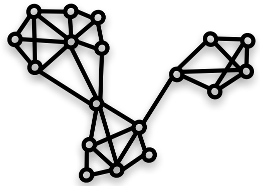
[17] Henaff, Bruna, LeCun 2015

Outline

➢ Part 1: Euclidean ConvNets
- *Architecture*
- *Non-Euclidean data*



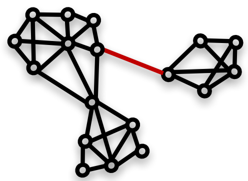
➢ **Part 2: Spectral ConvNets for Fixed Graphs**



➢ Spectral Graph Theory
- *Graph convolution*
- *Graph coarsening*

➢ **Spectral ConvNets**
- *SplineNets*
- *ChebNets* [NIPS'16]*
- *GraphConvNets*
- *CayleyNets**
- *Multiple fixed graphs* [NIPS'17]*

➢ Part 3: ConvNets for Variable Graphs
- *Graph learning problems**



➢ Conclusion

Spectral polynomial filters

- Represent smooth spectral functions with polynomials of Laplacian eigenvalues:

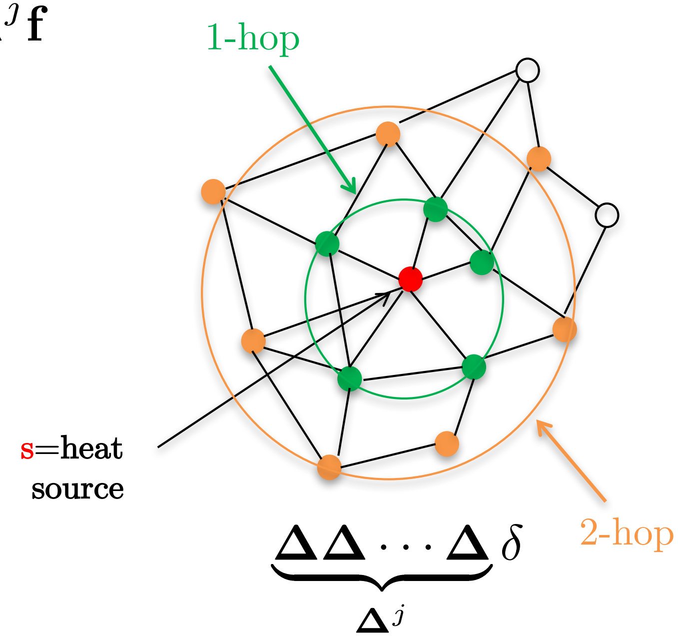
$$w_{\boldsymbol{\alpha}}(\lambda) = \sum_{j=0}^{r} \alpha_j \lambda^j$$

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 $\Rightarrow$ 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 ⇒ 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, ϕ$^\top$ ⇒ O(n) computational complexity (assuming sparsely-connected graphs)

☹ Unstable under coefficients perturbation (hard to optimize)

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

[18] Defferrard, Bresson, Vandergheynst 2016

Chebyshev polynomials

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

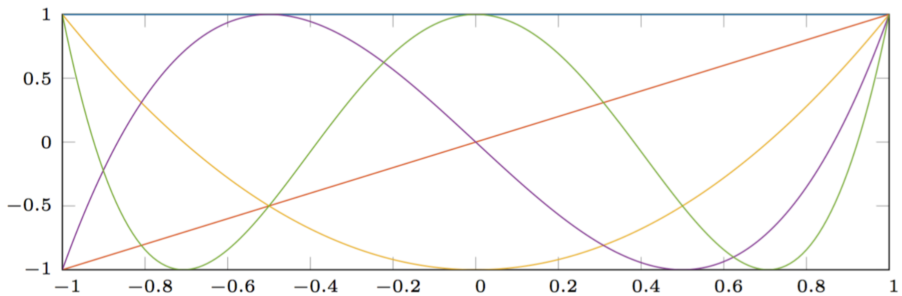
$$w_{\boldsymbol{\alpha}}(\boldsymbol{\Delta})\mathbf{f} = \sum_{j=0}^{r} \alpha_j \boldsymbol{\Delta}^j \mathbf{f}$$

- **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

- 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, $\phi^\top \Rightarrow O(n)$ computational complexity (assuming sparsely-connected graphs)

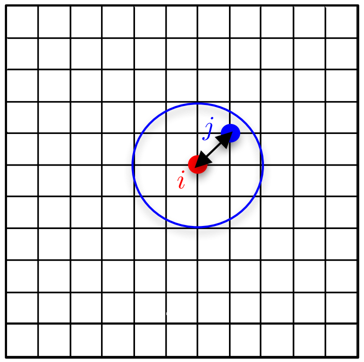
☺ Stable under coefficients perturbation

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

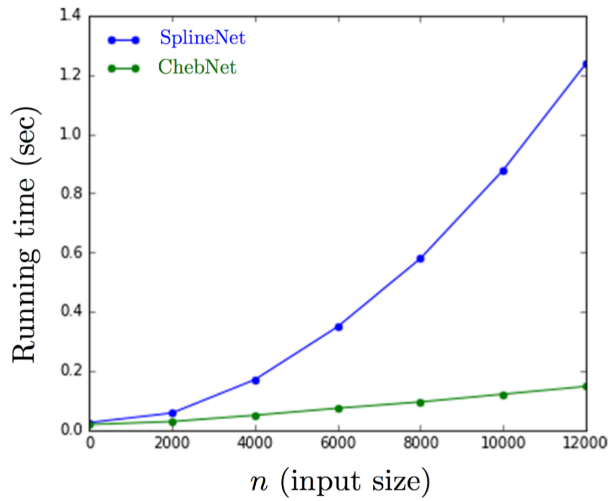
[18] Defferrard, Bresson, Vandergheynst 2016

Numerical experiments

Graph: a 8-NN graph of the Euclidean grid



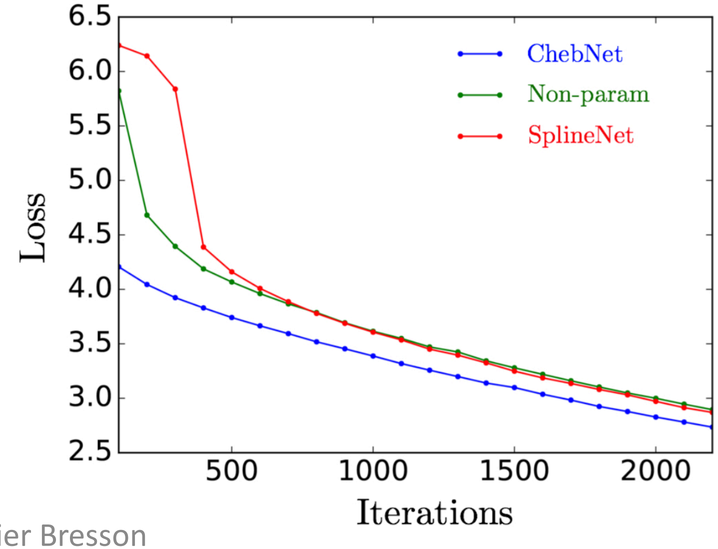
- **Running time**

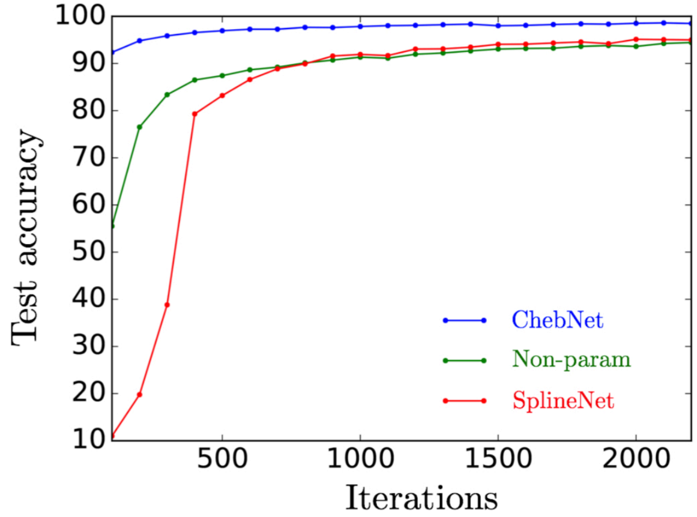


- **Accuracy**

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

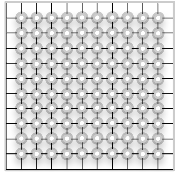
- **Optimization**



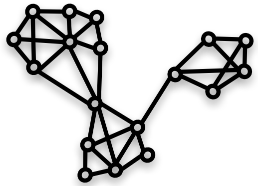


Outline

- Part 1: Euclidean ConvNets
  - *Architecture*
  - *Non-Euclidean data*

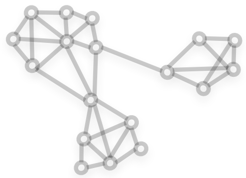


- **Part 2: Spectral ConvNets for Fixed Graphs**



  - Spectral Graph Theory
    - *Graph convolution*
    - *Graph coarsening*
  - **Spectral ConvNets**
    - *SplineNets*
    - *ChebNets* [NIPS'16]*
    - ***GraphConvNets***
    - *CayleyNets**
    - *Multiple fixed graphs* [NIPS'17]*

- Part 3: ConvNets for Variable Graphs
  - *Graph learning problems**



- Conclusion

Graph convolutional nets: 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

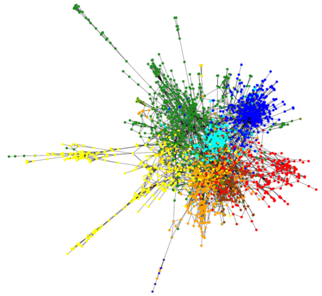
- Fix: Apply a renormalization

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

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

[19] Kipf, Welling 2016

Example: Citation networks



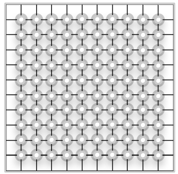
Method	Cora[1]	PubMed[2]
Manifold Regularization[3]	59.5%	70.7%
Semidefinite Embedding[4]	59.0%	71.1%
Label Propagation[5]	68.0%	63.0%
DeepWalk[6]	67.2%	65.3%
Planetoid[7]	75.7%	77.2%
Graph Convolutional Net[8]	**81.59%**	**78.72%**

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

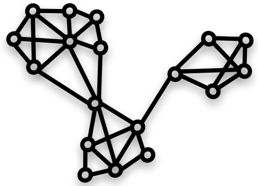
Outline

➢ Part 1: Euclidean ConvNets



- *Architecture*
- *Non-Euclidean data*

➢ **Part 2: Spectral ConvNets for Fixed Graphs**



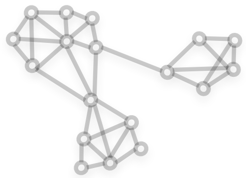
➢ Spectral Graph Theory

- *Graph convolution*
- *Graph coarsening*

➢ Spectral ConvNets

- *SplineNets*
- *ChebNets* [NIPS'16]*
- *GraphConvNets*
- *CayleyNets**
- *Multiple fixed graphs* [NIPS'17]*

➢ Part 3: ConvNets for Variable Graphs



- *Graph learning problems**

➢ Conclusion

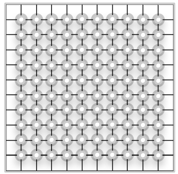
CayleyNets

Federico Monti (Universita della Svizzera Italiana)

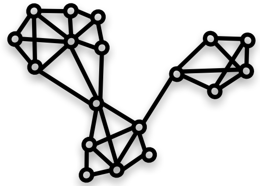
Deep Geometric Matrix Completion: a Geometric Deep Learning approach to Recommender Systems

Thursday, February 8, 2018, 10:10 - 10:50

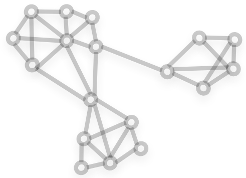
Outline



- Part 1: Euclidean ConvNets
  - *Architecture*
  - *Non-Euclidean data*



- **Part 2: Spectral ConvNets for Fixed Graphs**
  - Spectral Graph Theory
    - *Graph convolution*
    - *Graph coarsening*
  - Spectral ConvNets
    - *SplineNets*
    - *ChebNets* [NIPS'16]*
    - *GraphConvNets*
    - *CayleyNets**
    - *Multiple fixed graphs* [NIPS'17]*



- Part 3: ConvNets for Variable Graphs
  - *Graph learning problems**

- Conclusion

Spectral ConvNets for multiple fixed graphs

Federico Monti (Universita della Svizzera Italiana)

Deep Geometric Matrix Completion: a Geometric Deep Learning approach to Recommender Systems

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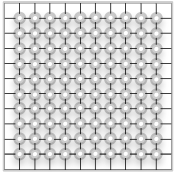
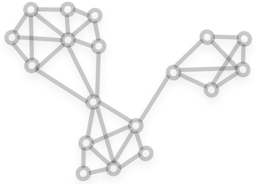
Outline

- Part 1: Euclidean ConvNets
  - *Architecture*
  - *Non-Euclidean data*



- Part 2: Spectral ConvNets for Fixed Graphs



  - Spectral Graph Theory
    - *Graph convolution*
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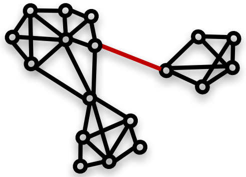
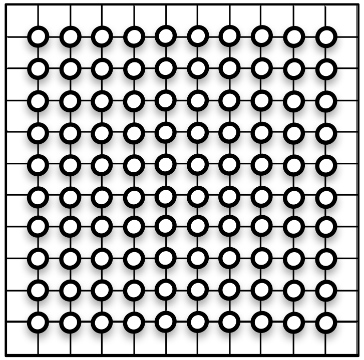
    - *GraphConvNets*
    - *CayleyNets**
    - *Multiple fixed graphs* [NIPS'17]*

- **Part 3: ConvNets for Variable Graphs**
  - *Graph learning problems**

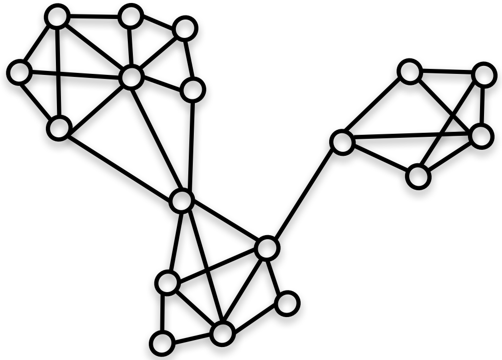


- Conclusion

Data domains



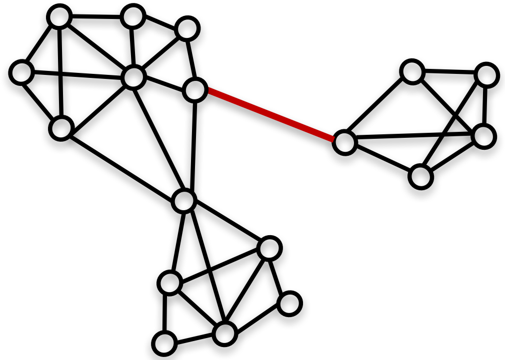
Euclidean
space/grid



Non-Euclidean
space/graph

Fixed domain

$\Rightarrow$



Change one single
edge

Variable domain

Standard
ConvNets

Spectral graph
ConvNets

Can we still use
spectral graph
ConvNets?

Spectral NNs offer rich
families of spectral filters

$\Rightarrow$

Are spectral filters
transferable?

Limitations of spectral NN techniques

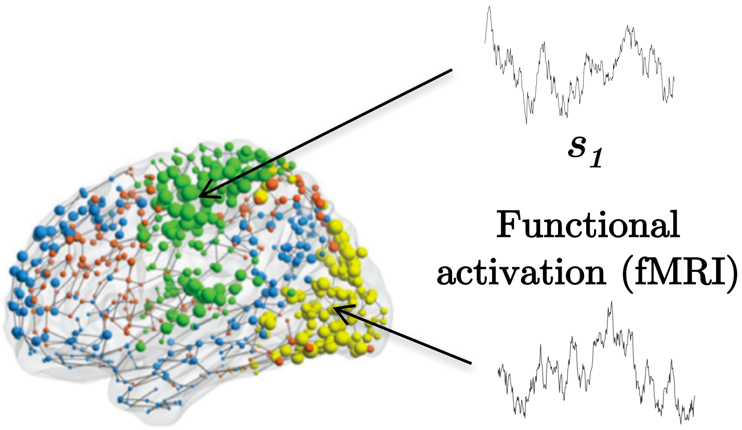
- Poor generalization to new/different graphs: Fourier modes are unstable under graph perturbations $\Rightarrow$ bad transfer/generalization of learned filters to new graphs:

$$\mathbf{\Phi}_{\mathcal{G}_1}\mathbf{W}\mathbf{\Phi}_{\mathcal{G}_1}^\top \mathbf{f} \neq \mathbf{\Phi}_{\mathcal{G}_2}\mathbf{W}\mathbf{\Phi}_{\mathcal{G}_2}^\top \mathbf{f}$$

- Aligning Fourier modes is hard, and does not guarantee good generalization.
- Directed graphs: Definition of directed graph Laplacian is unclear.
- Graphs with variable size: Spectral techniques work with fixed size graphs.

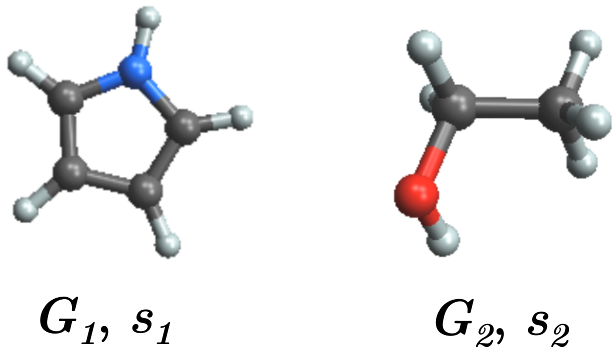
Problem setting

- **Spectral ConvNets:** Given fixed graph(s) G, and a set of signals s_k on G to be analyzed with ConvNets:



Brain connectivity network (sMRI)
Fixed graph G

- **ConvNets for arbitrary graphs:** Given a set of graphs G_k and signals s_k on G_k to be analyzed with ConvNets:

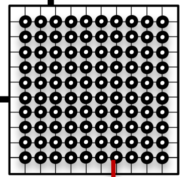


Molecules
Variable graphs G_k

Graph ConvNet architectures

Signal s_k: Image

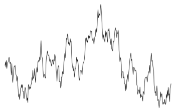
Part 1:
(Standard)
ConvNets



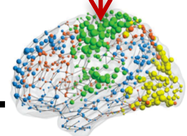
Classification

New data
domain

Signal s_k: fMRI



Part 2:
Spectral
ConvNets

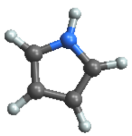


Classification

Fixed graph G

New data
domain

Signal s_k on graph G_k:
Molecule with atoms



Part 3:
Graph
ConvNets

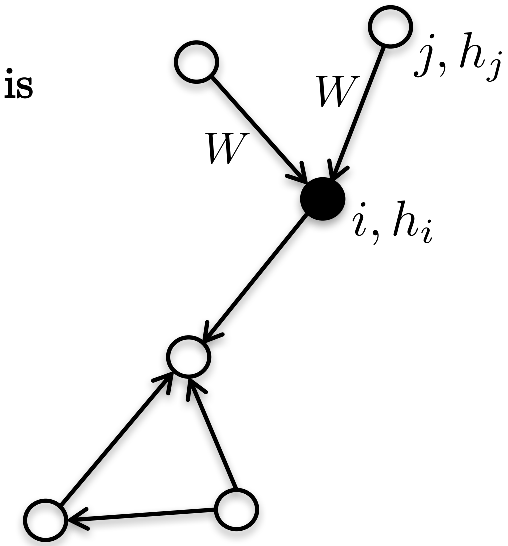
Classification

Variables graphs G_k

Graph neural networks

- Spatial NN technique to deal with arbitrary graphs[27].

- Minimal inner structures:
  - Invariant by vertex re-indexing (no graph matching is required)
  - Locality (only neighbors are considered)
  - Weight sharing (convolutional operations)
  - Independence w.r.t. graph size



$$h_i = f_{\text{GNN}}\left(\{h_j : j \to i\}\right)$$

- What instantiation of f ?

[27] Scarselli et-al 2009

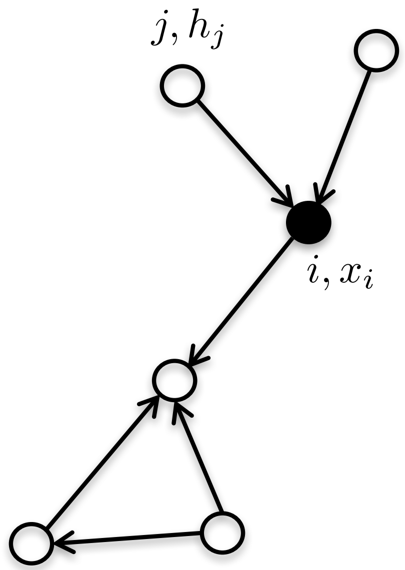
Graph RNNs

- **Graph RNN: Multilayer perceptron**[27]

$$h_i = \sum_{j \to i} \mathcal{C}_{\text{G-MLP}}(x_i, h_j) = \sum_{j \to i} A\sigma(B\sigma(Ux_i + Vh_j))$$

- **Graph GRU**[28,29] **(Gated Recurrent Unit)**

$$h_i = \mathcal{C}_{\text{G-GRU}}(x_i, \sum_{j \to i} h_j)$$



Fixed-point iterative scheme:

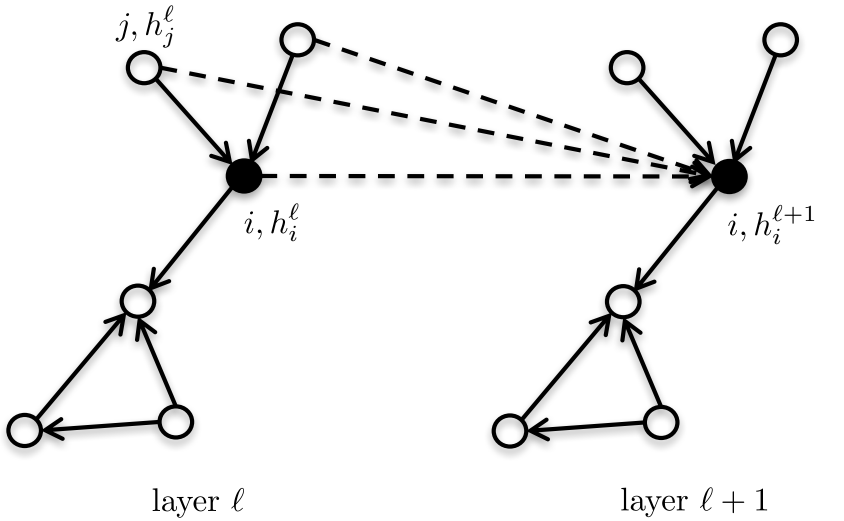
$$\begin{aligned}
\bar{h}_i^t &= \sum_{j \to i} h_j^t, \quad h_i^{t=0} = x_i \\
z_i^{t+1} &= \sigma(U_z h_i^t + V_z \bar{h}_i^t) \\
r_i^{t+1} &= \sigma(U_r h_i^t + V_r \bar{h}_i^t) \\
\tilde{h}_i^{t+1} &= \tanh\big(U_h(h_i^t \odot r_i^{t+1}) + V_h \bar{h}_i^t\big) \\
h_i^{t+1} &= (1 - z_i^{t+1}) \odot h_i^t + z_i^{t+1} \odot \tilde{h}_i^{t+1}
\end{aligned}$$

[27] Scarselli et-al 2009
[28] Li, Tarlow, Brockschmidt, Zemel, 2015
[29] Cho et-al, 2014

Graph ConvNets

- **Vanilla graph ConvNets[30]:**

$$
\begin{aligned}
h_i^{\ell+1} &= \mathcal{C}_{\text{G-VCN}}\Big(h_i^\ell, \sum_{j\to i} h_j^\ell\Big), \quad h_i^{\ell=0} = x_i \\
&= \mathrm{ReLU}\Big(U^\ell h_i^\ell + V^\ell \sum_{j\to i} h_j^\ell\Big), \quad h_i^{\ell=0} = x_i
\end{aligned}
$$



[30] Sukhbaatar, Szlam, Fergus 2016

Sainaa Sukhbaatar (New York University)

Deep Architecture for Sets and Its Application to
Multi-agent Communication

Friday, February 9, 2018, 9:00 - 9:40

Graph RNNs or ConvNets?

- Common trend: Most published papers use RNN architectures (GRU, LSTM) $\Rightarrow$ Are they superior to ConvNet architectures for arbitrary graphs?

- Numerical study to compare both graph architectures[31] for 2 basic and representative graph problems:
  - Subgraph matching[27]
  - Semi-supervised classification

[27] Scarselli et-al 2009
[31] Bresson, Laurent 2017

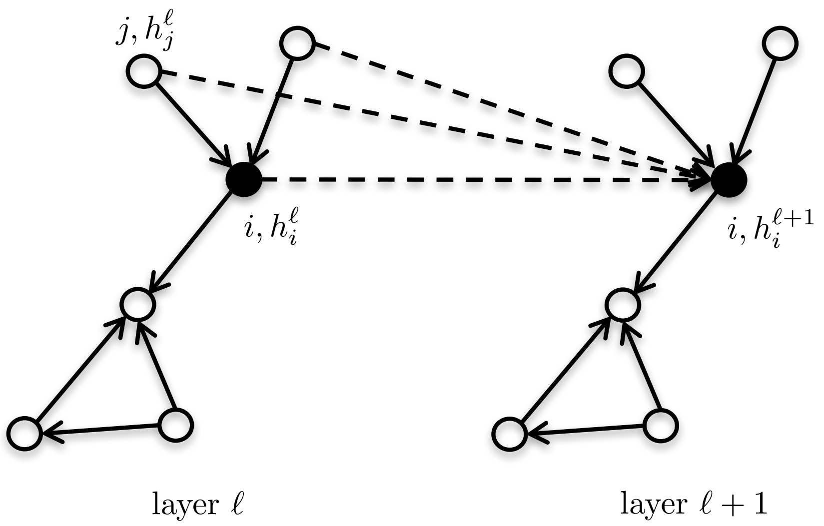
Gated graph ConvNets

- Graph ConvNets architecture with edge gating mechanism (leveraging[30,32,33]) and residuality[31]:

$$h_i^{\ell+1} = \mathrm{ReLU}\left(U^\ell h_i^\ell + \sum_{j \to i} \eta_{ij} \odot V^\ell h_j^\ell \right)$$

edge gates
(anisotropic property)

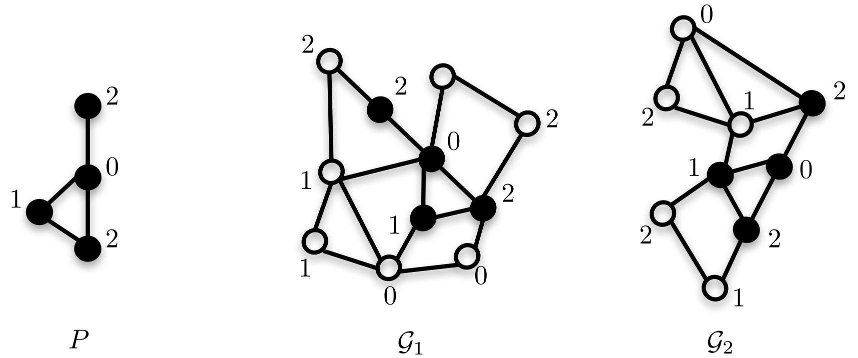
$$\eta_{ij} = \sigma\left(A^\ell h_i^\ell + B^\ell h_j^\ell \right)$$



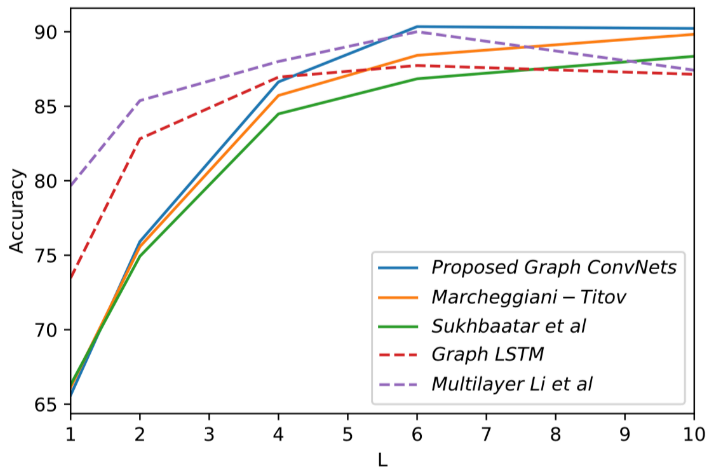
[31] Bresson, Laurent 2017
[30] Sukhbaatar, Szlam, Fergus 2016
[32] Tai, Socher, Manning, 2015
[33] Marcheggiani, Titov 2017

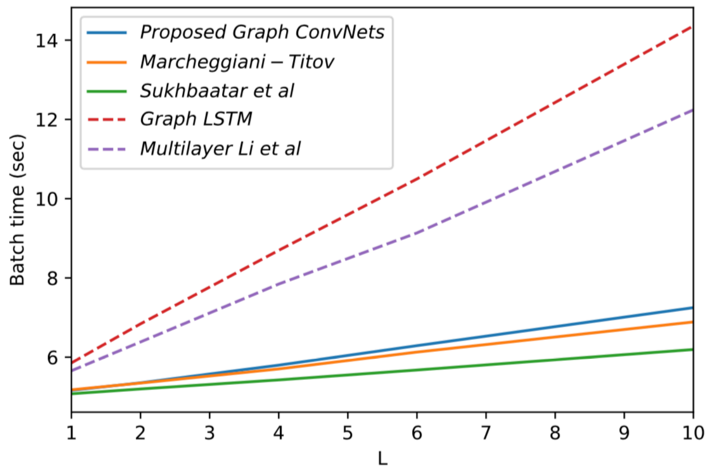
Graph learning problem 1

- Pattern matching



- Experimental results:



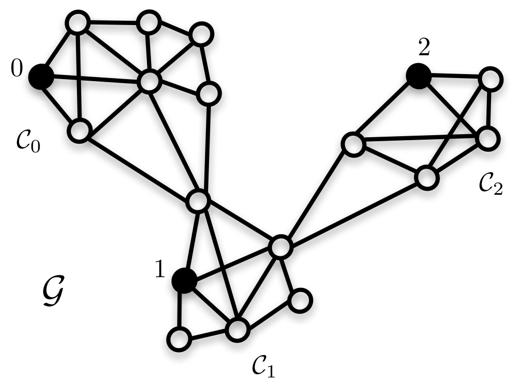


- All graph NNs are upgraded with residuality (offers 10% improvements).

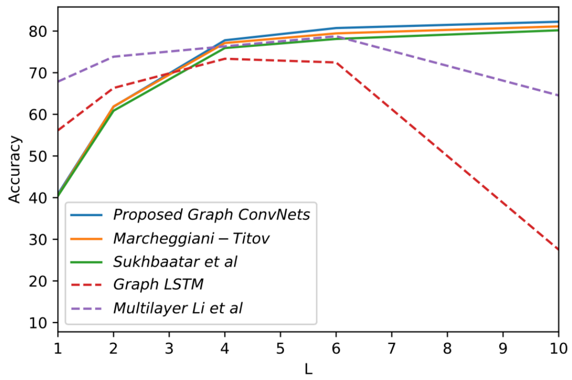
[31] Bresson, Laurent 2017

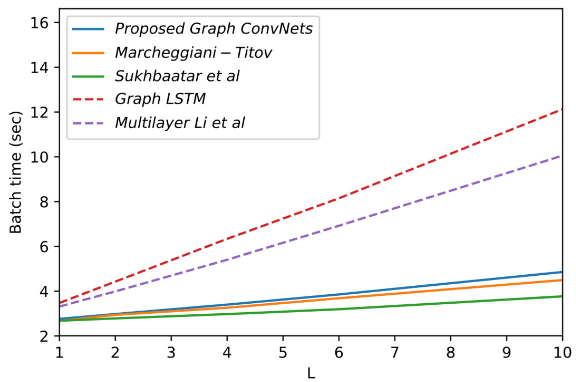
Graph learning problem 2

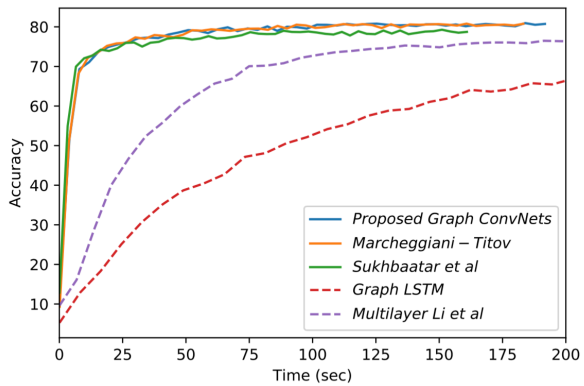
- **Semi-supervised clustering**



- **Experimental results:**



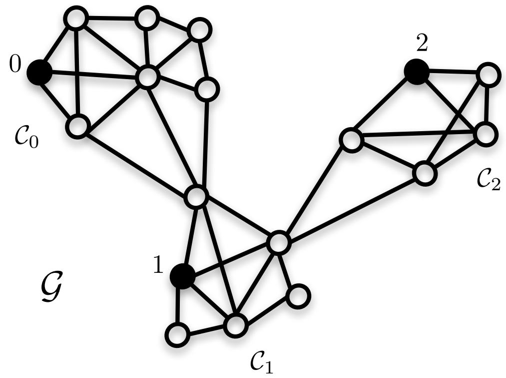




- **Conclusion:** Use ConvNets architecture for variable graphs.

Learning vs. non-learning techniques

- Semi-supervised clustering

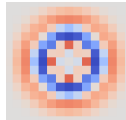


- Comparing learning vs non-learning (variational) techniques[34]: 82% vs 45% and test time is $O(E)$ vs $O(E^{3/2})$.

[34] Grady 2006

Remarks

- Anisotropy vs isotropy:
  - Standard ConvNets produce anisotropic filters because Euclidean grids have directional structure.
  - Graph ConvNets compute isotropic filters because there is no notion of directions on arbitrary graphs.
  - How to get anisotropy back for graphs?
    - Edge gates[31]/attention[36] information to treat neighbors differently.
    - Differentiate graph edges and graph vertices[35] (e.g. different atoms and atom connections)

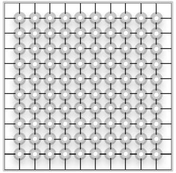


- Graph learning:
  - For social networks, brain connectivity, road network, the graph is fixed and given.
  - For citations network, image network, NLP, the graph must be constructed/learned.

[31] Bresson, Laurent 2017
[35] Gilmer et-al 2017
[36] Velickovic et-al 2017

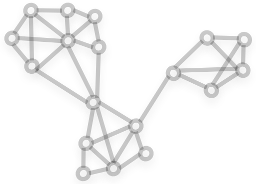
Outline

- Part 1: Euclidean ConvNets



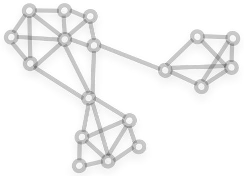
  - *Architecture*
  - *Non-Euclidean data*

- Part 2: Spectral ConvNets for Fixed Graphs



  - Spectral Graph Theory
    - *Graph convolution*
    - *Graph coarsening*
  - Spectral ConvNets
    - *SplineNets*
    - *ChebNets* [NIPS'16]*
    - *GraphConvNets*
    - *CayleyNets**
    - *Multiple fixed graphs* [NIPS'17]*

- Part 3: ConvNets for Variable Graphs



  - *Graph learning problems**

- **Conclusion**

Conclusion

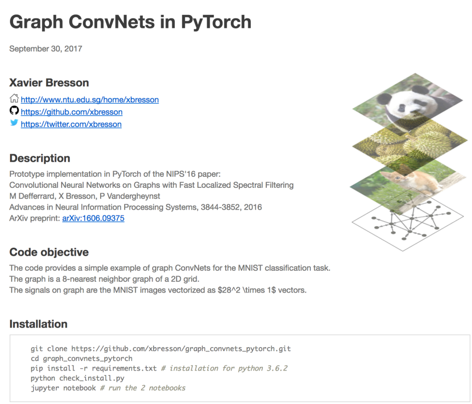
- Contributions:
  - Generalization of ConvNets to data on graphs
  - Exact/tight localized filters on graphs
  - Linear complexity for sparse graphs
  - GPU implementation
  - Rich expressivity
  - Multiple and arbitrary graphs

- Several potential applications in data and network sciences.

Papers and codes

- Papers
  - Convolutional neural networks on graphs with fast localized spectral filtering, M Defferrard, X Bresson, P Vandergheynst, NIPS, 2016, arXiv:1606.09375
  - Geometric matrix completion with recurrent multi-graph neural networks, F Monti, MM Bronstein, X Bresson, NIPS, 2017, arXiv:1704.06803
  - CayleyNets: Graph Convolutional Neural Networks with Complex Rational Spectral Filters, R Levie, F Monti, X Bresson, MM Bronstein, 2017, arXiv:1705.07664
  - Residual Gated Graph ConvNets, X Bresson, T Laurent, 2017, arXiv:1711.07553

- Codes
  - https://github.com/xbresson/graph_convnets_pytorch



Graph ConvNets in PyTorch

September 30, 2017

Xavier Bresson

http://www.ntu.edu.sg/home/xbresson
https://github.com/xbresson
https://twitter.com/xbresson

Description

Prototype implementation in PyTorch of the NIPS'16 paper:
Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering
M Defferrard, X Bresson, P Vandergheynst
Advances in Neural Information Processing Systems, 3844-3852, 2016
ArXiv preprint: arXiv:1606.09375

Code objective

The code provides a simple example of graph ConvNets for the MNIST classification task.
The graph is a 8-nearest neighbor graph of a 2D grid.
The signals on graph are the MNIST images vectorized as $28^2 \times 1$ vectors.

Installation

```
git clone https://github.com/xbresson/graph_convnets_pytorch.git
cd graph_convnets_pytorch
pip install -r requirements.txt # installation for python 3.6.2
python check_install.py
jupyter notebook # run the 2 notebooks
```

Thank you

http://www.ntu.edu.sg/home/xbresson
https://github.com/xbresson
https://twitter.com/xbresson