Deep Learning on Irregular Domains (DLID)

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Deep Learning on Graphs

Learning beyond Euclidean Data

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Structured data

Why structure data ?

- To incorporate additional information.
- To exploit spatial correlations.
- To decrease learning complexity by making geometric assumptions.

Data structured by Euclidean grids.

- 1D: sound, time-series.
- 2D: images.
- 3D: video, hyper-spectral images.

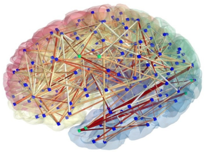
Naturally graph-structured data

Modeling versatility: graphs model heterogeneous pairwise relationships.

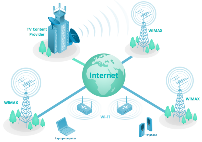
Examples of irregular / graph-structured data:

- Social networks: Facebook, Twitter.
- Biological networks: genes, molecules, brain connectivity.
- Infrastructure networks: energy, transportation, Internet, telephony.

Social network



Brain structure



Telecommunication

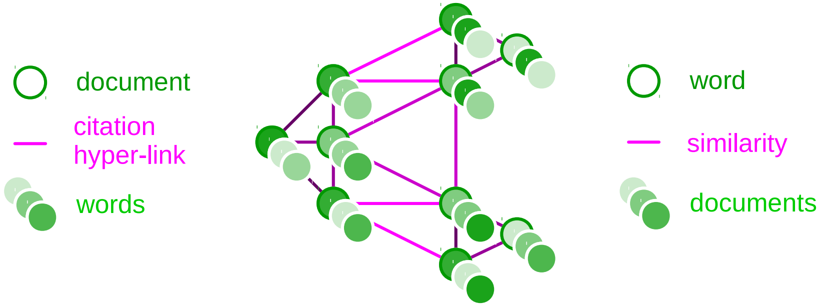
Types of graphs

Sample graph

- Semi-supervised learning.
- Incorporate external information.

Feature graph

- Reduce computations.
- Incorporate external information.



Problems: signals, nodes or graphs classification (regression).

Using the structure

Extrinsic: embed the graph in an Euclidean space.

- Each node is represented by a vector.
- Use that embedding as additional features for a fully connected NN.
- Use a convolutional NN in the embedding space.
  Possibly very high-dimensional!

Intrinsic: a Neural Net defined on graphically structured data.

- Exploit geometric structure for computational efficiency.
- Starting point: ConvNet, an intrinsic formulation for Euclidean grids.

Why ConvNets?

ConvNets are extremely efficient at extracting meaningful statistical patterns in large-scale and high-dimensional datasets.

They exploit the geometry.

Statistical assumptions

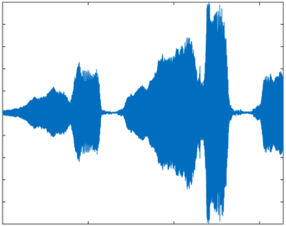
- Localization: compact filters for low complexity.
- Stationarity: translation invariance.
- Compositionality: analysis with a filterbank.
- Multi-scale: hierarchical features extracted by multiple layers.

Developed for data lying on Euclidean grids

All operations are well defined and computationally efficient:

1. Convolution $\rightarrow$ filter translation or fast Fourier transform (FFT).
2. Down-sampling $\rightarrow$ pick one pixel out of n.
3. Non-linearity $\rightarrow$ point-wise operation.
4. Pooling $\rightarrow$ summarize the receptive field.

Image (2D) Video (3D)

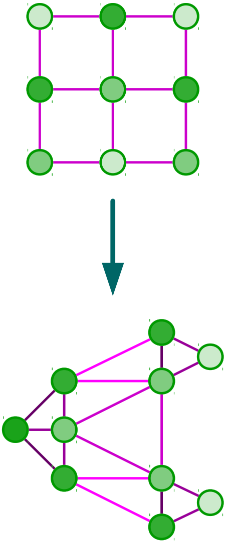


Sound (1D)

ConvNets on graphs

Graphs vs Euclidean grids

- Irregular sampling.
- Weighted edges.
- No orientation (in general).



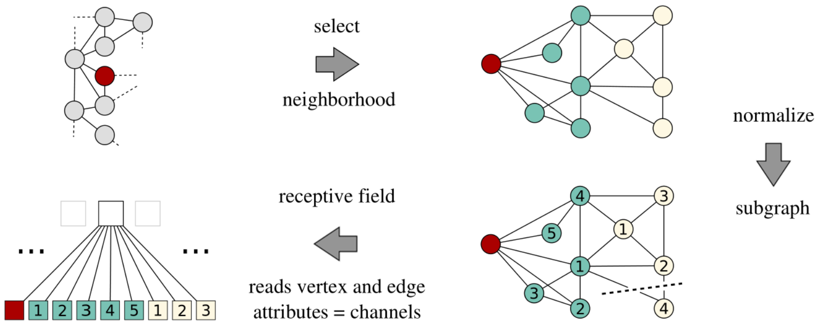
Challenges

1. Formulate convolution and down-sampling on graphs.
2. Make them efficient!

ConvNets on graphs: spatial approach

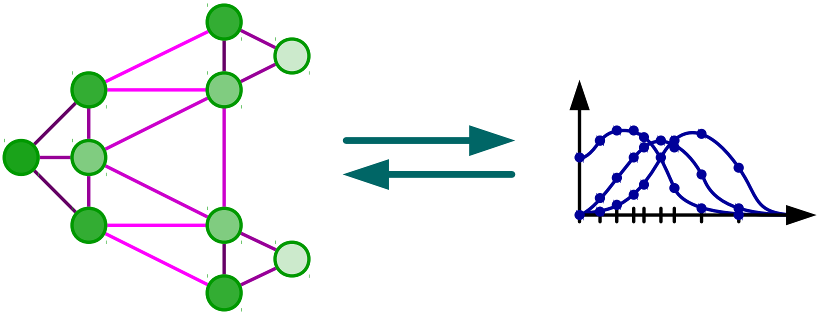
Niepert, Ahmed, and Kutzkov 2016

1. Define receptive field / neighborhood.
2. Order nodes, i.e. give orientations to a node's edges.



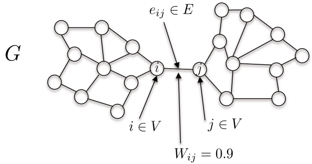
ConvNets on graphs: spectral approach

Bruna, Zaremba, Szlam, and LeCun 2014; Henaff, Bruna, and LeCun 2015



Graphs

$\mathcal{G} = (\mathcal{V}, \mathcal{E}, W)$: undirected and connected graph



- $\mathcal{V}$: set of $|\mathcal{V}| = n$ vertices
- $\mathcal{E}$: set of edges
- $W \in \mathbb{R}^{n \times n}$: weighted adjacency matrix
- $D_{ii} = \sum_j W_{ij}$: diagonal degree matrix

Graph Laplacians (core operator to spectral graph theory):

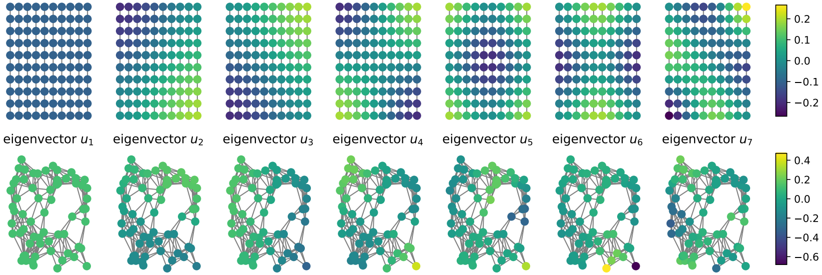
- $L = D - W \in \mathbb{R}^{n \times n}$: combinatorial
- $L = I_n - D^{-1/2} W D^{-1/2}$: normalized

Graph Fourier basis

Shuman, Narang, Frossard, Ortega, and Vandergheynst 2013

L is symmetric and positive semidefinite $\rightarrow L = U \Lambda U^T$ (EVD)

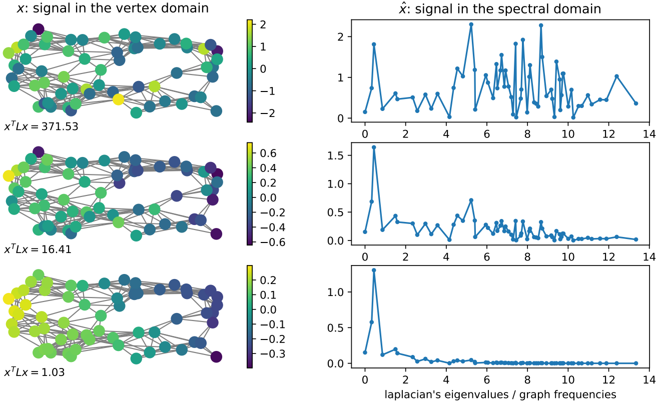
- Graph Fourier basis $U = [u_1, \ldots, u_n] \in \mathbb{R}^{n \times n}$
- Graph "frequencies" $\Lambda = \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} \in \mathbb{R}^{n \times n}$



Graph Fourier Transform

Shuman, Narang, Frossard, Ortega, and Vandergheynst 2013

- Graph signal $x : \mathcal{V} \to \mathbb{R}$ seen as $x \in \mathbb{R}^n$
- Transform: $\hat{x} = \mathcal{F}_{\mathcal{G}}\{x\} = U^T x \in \mathbb{R}^n$
- Inverse: $x = \mathcal{F}_{\mathcal{G}}^{-1}\{x\} = U\hat{x} = UU^T x = x$

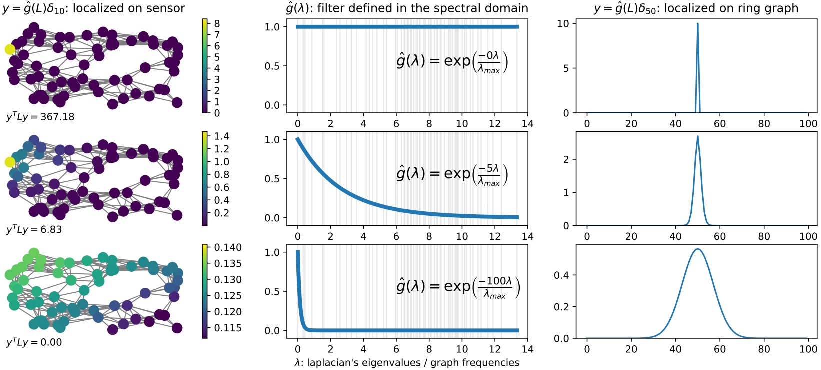


Filtering with convolution on graphs

Shuman, Narang, Frossard, Ortega, and Vandergheynst 2013

Convolution theorem: $y = x *_{\mathcal{G}} g = U\left(U^T g \odot U^T x\right) = U\left(\hat{g} \odot U^T x\right)$

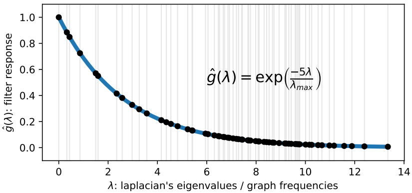
$$y = x *_{\mathcal{G}} g = U \begin{bmatrix} \hat{g}(\lambda_0) & & 0 \\ & \ddots & \\ 0 & & \hat{g}(\lambda_{n-1}) \end{bmatrix} U^T x = U \hat{g}(\Lambda) U^T x = \hat{g}(L) x$$



Spectral filtering of graph signals

Non-parametric filter, can learn all possible filters:

$$\hat{g}_\theta(\Lambda) = \mathrm{diag}(\theta),\ \theta \in \mathbb{R}^n$$



- Non-localized in vertex domain
- Learning complexity in $\mathcal{O}(n)$
- Computational complexity in $\mathcal{O}(n^2)$ (& memory)

Variation: a smooth function such as $\hat{g}_\theta(\Lambda) = B\theta$ where B is the cubic spline basis (Bruna, Zaremba, Szlam, and LeCun 2014).

Polynomial parametrization

Shuman, Ricaud, and Vandergheynst 2016

$$\hat{g}_\theta(\Lambda) = \sum_{k=0}^{K-1} \theta_k \Lambda^k, \ \theta \in \mathbb{R}^K$$

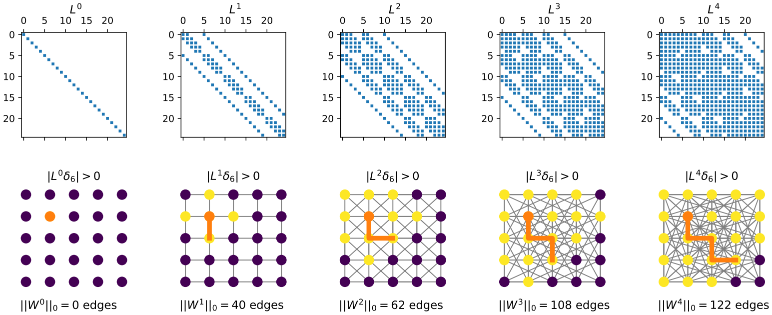
- Can learn all K-localized filters.
- Distributed computing: only need access to the K-neighborhood.

- K-localized
- Learning complexity in $\mathcal{O}(K)$
- Computational complexity in $\mathcal{O}(n^2)$

Filter localization

Hammond, Vandergheynst, and Gribonval 2011, Lemma 5.2

- Value at j of g_θ centered at i: $(\hat{g}_\theta(L)\delta_i)_j = (\hat{g}_\theta(L))_{i,j} = \sum_k \theta_k (L^k)_{i,j}$
- $d_\mathcal{G}(i,j) > K$ implies $(L^K)_{i,j} = 0$



Filter localization

Shuman, Ricaud, and Vandergheynst 2016

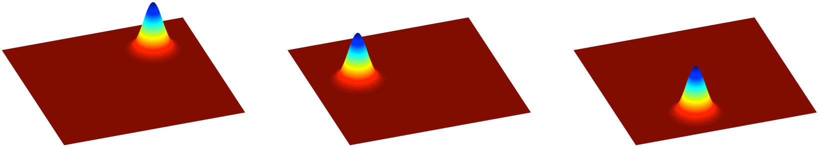


Figure: Localization on regular Euclidean grid.

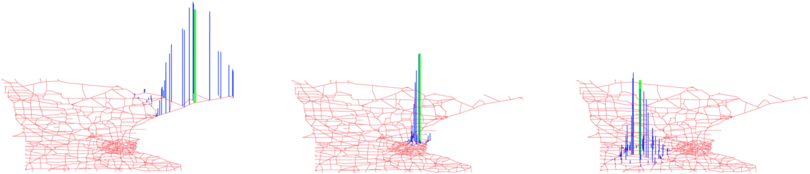


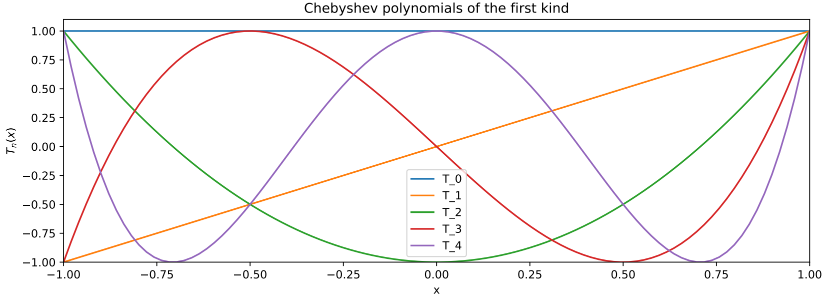
Figure: Localization on graph with $(\hat{g}_\theta(L)\delta_i)_j = (\hat{g}_\theta(L))_{i,j}$.

Recursive formulation with Chebyshev polynomials

Hammond, Vandergheynst, and Gribonval 2011

$$\hat{g}_\theta(\Lambda) = \sum_{k=0}^{K-1} \theta_k T_k(\tilde{\Lambda}), \quad \tilde{\Lambda} = 2\lambda_n^{-1}\Lambda - I_n$$

Chebyshev polynomials: $T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$ with $T_0 = 1$ and $T_1 = x$



Recursive formulation with Chebyshev polynomials

$$y = \hat{g}_\theta(L)x = \sum_{k=0}^{K-1} \theta_k T_k(\tilde{L})x, \quad \tilde{L} = 2\lambda_n^{-1} L - I_n$$

Recurrence:

$$\begin{aligned} y &= \hat{g}_\theta(L)x = [\bar{x}_0, \ldots, \bar{x}_{K-1}]\theta \\ \bar{x}_k &= T_k(\tilde{L})x = 2\tilde{L}\bar{x}_{k-1} - \bar{x}_{k-2} \\ \bar{x}_0 &= x \\ \bar{x}_1 &= \tilde{L}x \end{aligned}$$

- K-localized
- Learning complexity in $\mathcal{O}(K)$
- Computational complexity in $\mathcal{O}(K|\mathcal{E}|)$ (same as classical ConvNets!)

Learning filters

Defferrard, Bresson, and Vandergheynst 2016

$$y_{s,j} = \sum_{i=1}^{F_{in}} \hat{g}_{\theta_{i,j}}(L) x_{s,i} \in \mathbb{R}^n$$

- $x_{s,i}$: feature map i of sample s
- $\theta_{i,j}$: trainable parameters
  ($F_{in} \cdot F_{out}$ vectors of K Chebyshev coefficients)

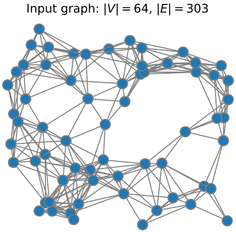
Gradients for backpropagation:

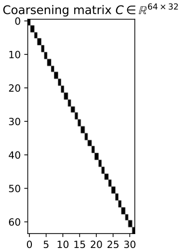
- $\frac{\partial E}{\partial \theta_{i,j}} = \sum_{s=1}^{S} [\bar{x}_{s,i,0}, \ldots, \bar{x}_{s,i,K-1}]^T \frac{\partial E}{\partial y_{s,j}}$
- $\frac{\partial E}{\partial x_{s,i}} = \sum_{j=1}^{F_{out}} g_{\theta_{i,j}}(L) \frac{\partial E}{\partial y_{s,j}}$

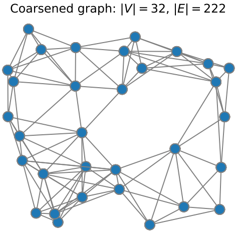
Overall cost of $\mathcal{O}(K|\mathcal{E}|F_{in}F_{out}S)$ operations, $|\mathcal{E}| \propto n$ for sparse graphs

Coarsening

Defferrard, Bresson, and Vandergheynst 2016



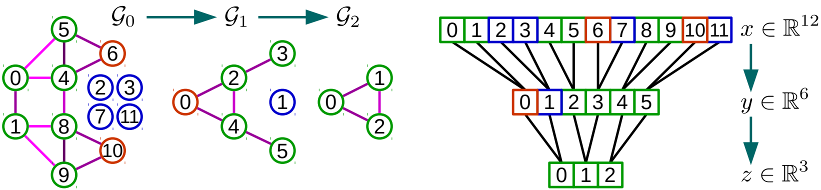




- Inherently combinatorial problem.
- Can be done as pre-processing.
- Greedy node merging with Graclus / Metis (very fast).

Pooling

Defferrard, Bresson, and Vandergheynst 2016

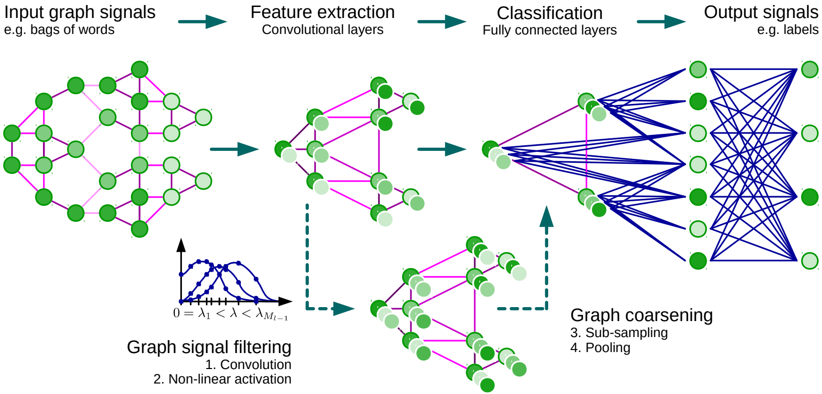


Pooling as any regular 1D signal

- Node order does not matter $\rightarrow$ arrange them for local access.
- Nodes at multiple levels are ordered as a tree.
- Satisfies parallel architectures like GPUs.

Graph ConvNet architecture

Defferrard, Bresson, and Vandergheynst 2016



Revisiting MNIST

Model	Architecture	Accuracy
Classical CNN	C32-P4-C64-P4-FC512	99.33
Proposed graph CNN	GC32-P4-GC64-P4-FC512	99.14

Table: Comparison to classical ConvNets.

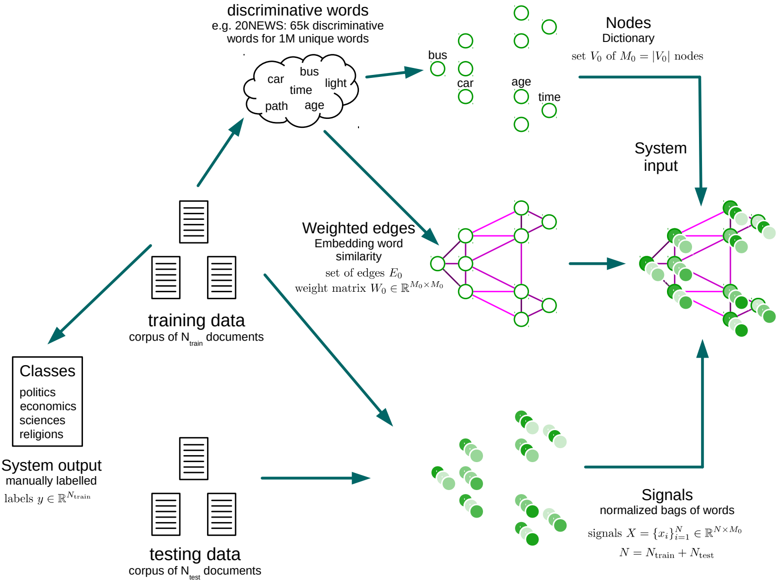
Comparable to classical ConvNets,
and better than other parametrizations!

	Accuracy		
Architecture	Non-Param	Spline	Chebyshev
GC10	95.75	97.26	97.48
GC32-P4-GC64-P4-FC512	96.28	97.15	99.14

Table: Comparison between spectral filters, $K = 25$.

20NEWS: structuring documents with a feature graph

Defferrard, Bresson, and Vandergheynst 2016



Classification accuracy & Graph quality

Model	Accuracy
Linear SVM	65.90
Multinomial Naive Bayes	68.51
Softmax	66.28
FC2500	64.64
FC2500-FC500	65.76
GC32	68.26

Proposed graph CNN vs. other methods on 20NEWS.

	word2vec			
bag-of-words	pre-learned	learned	approximate	random
67.50	66.98	68.26	67.86	67.75

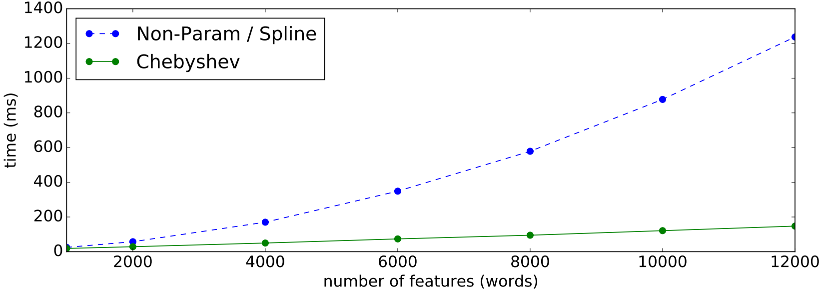
Different graphs on 20NEWS.

Architecture	8-NN on 2D Euclidean grid	random
GC32	97.40	96.88
GC32-P4-GC64-P4-FC512	99.14	95.39

Different graphs on MNIST.

20NEWS: training time

Defferrard, Bresson, and Vandergheynst 2016



Make CNNs practical for graph signals!

Spline: $\hat{g}_\theta(\Lambda) = B\theta$ where B is the cubic spline basis
(Bruna, Zaremba, Szlam, and LeCun 2014)

Recurrent Graph Convolutional Network

Seo, Defferrard, Bresson, and Vandergheynst 2016

1D signals

- $h_t = \tanh(W_x x_t + W_h h_{t-1})$
- $y_t = W h_t$
- State stored in hidden units

Graph signals

- $h_t = \tanh(W_x *_{\mathcal{G}} x_t + W_h *_{\mathcal{G}} h_{t-1})$
- $y_t = W *_{\mathcal{G}} h_t$
- State stored locally on the nodes

- Graph filtering x as $y = [\bar{x}_0, \ldots, \bar{x}_{K-1}]\theta$ is a weighted sum of diffused versions $\bar{x}$ of x.
- Data exchanged locally around the K-neighborhood.
- Reduces to independent signals if $K = 1$ or graph has no edge.

Various applications

- Semi-supervized learning
  [Kipf and Welling 2016; Manessi, Rozza, and Manzo 2017]
- Quantum Chemistry
  [Duvenaud et al. 2015; Gilmer, Schoenholz, Riley, Vinyals, and Dahl 2017]
- High Energy Physics
- Computer Graphics [Monti, Boscaini, et al. 2016; Yi, Su, Guo, and Guibas 2016; Wang, Gan, Zhang, and Shui 2017; Simonovsky and Komodakis 2017]
- Community detection [Bruna and Li 2017]
- Brain analysis
  [Ktena et al. 2017; Parisot et al. 2017; Anirudh and Thiagarajan 2017]
- Matrix completion for recommendation
  [Monti, Bronstein, and Bresson 2017]
- Neural machine translation
  [Bastings, Titov, Aziz, Marcheggiani, and Sima'an 2017]
- Link prediction and entity classification in knowledge bases
  [Schlichtkrull et al. 2017]

Conclusion

- Many problems can be defined as data structured by graphs.
- ConvNets are efficient because they exploit the geometry.
- Spatial approaches require nodes to be ordered.
- Convolution is well-defined in the Fourier domain, though the graph Fourier transform (GFT) is expensive.
- Polynomial formulations of order K are K-localized and do not require the GFT.
- Graph coarsening is a research problem in itself.
- Pooling made efficient by ordering nodes and inserting fake nodes.
- Loss of edge orientation is not killing performance on images.
- Having a good (relative to the task) graph is important.
- RNN extension can accommodate structured time series.
- Many proposed applications and many more to come.

Thanks Questions?

- Paper: Defferrard, Bresson and Vandergheynst, Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering, NIPS, 2016.
- Code: `https://github.com/mdeff/cnn_graph`
- Paper: Seo, Defferrard, Bresson and Vandergheynst, Structured Sequence Modeling with Graph Convolutional Recurrent Networks, arXiv, 2017.
- Code: `https://github.com/youngjoo-epfl/gconvRNN`