Graph Signal Processing Workshop

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Deep Learning on Graphs

Learning beyond Euclidean Data

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Structured data

Majority of data is naturally unstructured.
But can be structured by graphs.

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.

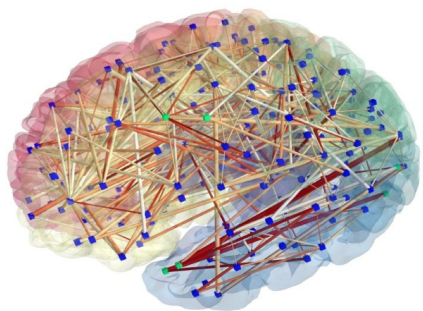
Non-Euclidean data: natural graphs

Modeling versatility: graphs model heterogeneous pairwise relationships.

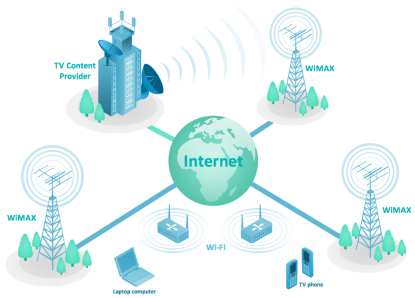
Examples of irregular / graph-structured data:

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

Social network



Brain structure



Telecommunication

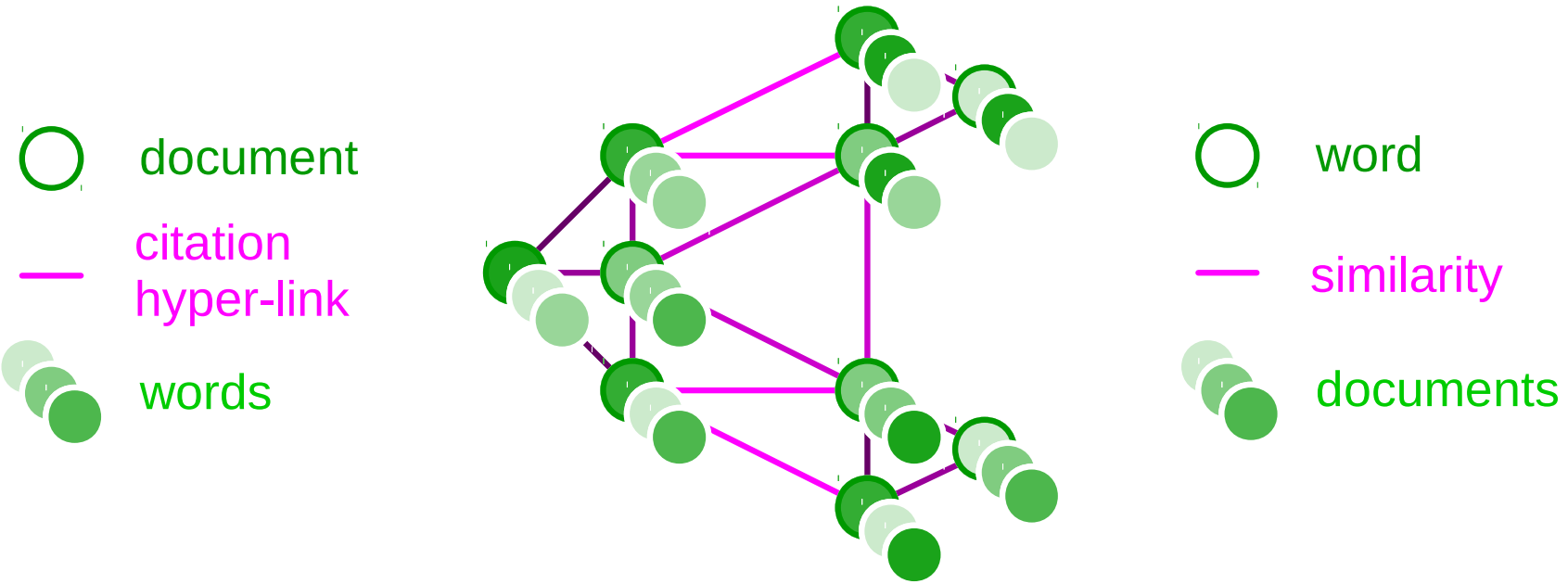
Non-Euclidean data: constructed graphs

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.

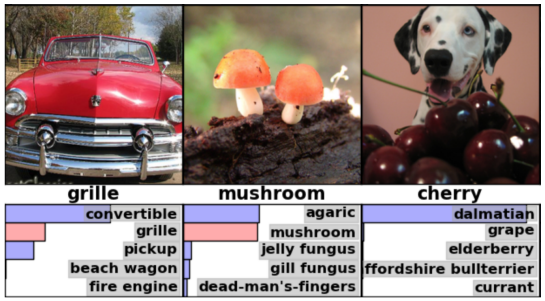
- Exploit geometric structure for computational efficiency.
- Starting point: ConvNet, an intrinsic formulation for Euclidean grids.

ConvNets are ubiquitous

LeCun, Bengio, and Hinton 2015

First developed for Computer Vision

- Object recognition
- Image captioning
- Image inpainting



Spreading outside CV

- Natural language processing
- Audio: sound & voice
- Autonomous agents (playing Atari or Go)

Why are ConvNets good ?

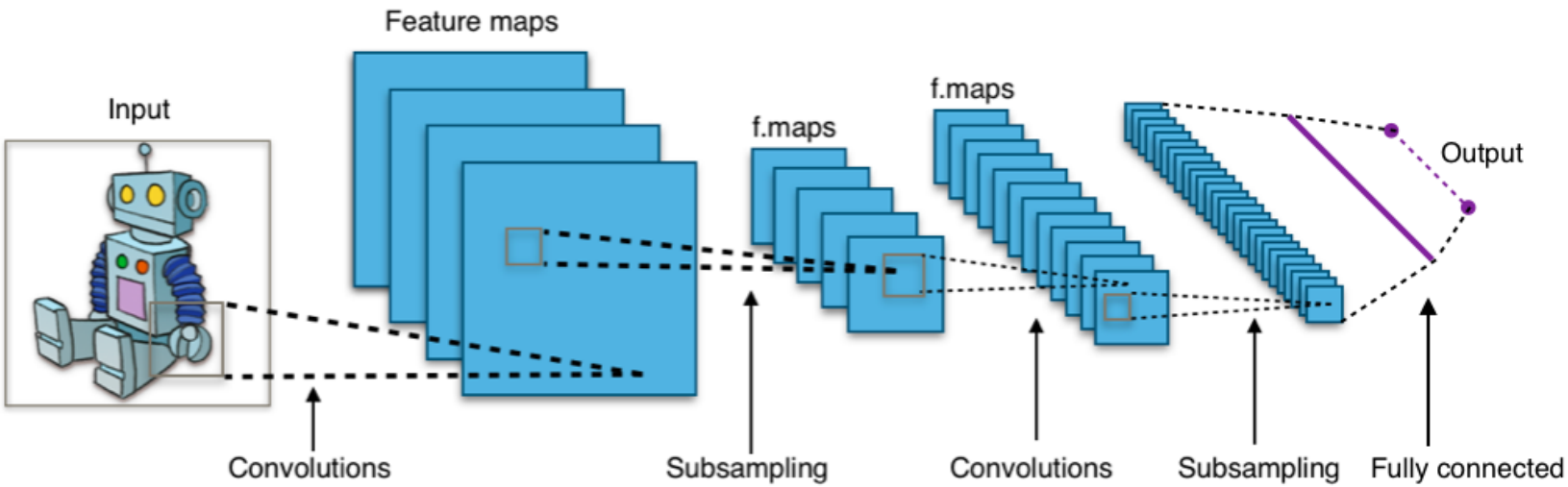
ConvNets are extremely efficient at extracting meaningful statistical patterns in large-scale and high-dimensional datasets.

They exploit the underlying geometric structure in the data.

Statistical assumptions

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

ConvNets: architecture



Ingredients

1. Convolution (local)
2. Non-linearity (point-wise)
3. Down-sampling (global / local)
4. Pooling (local)

ConvNets: feature extraction

Zeiler and Fergus 2014

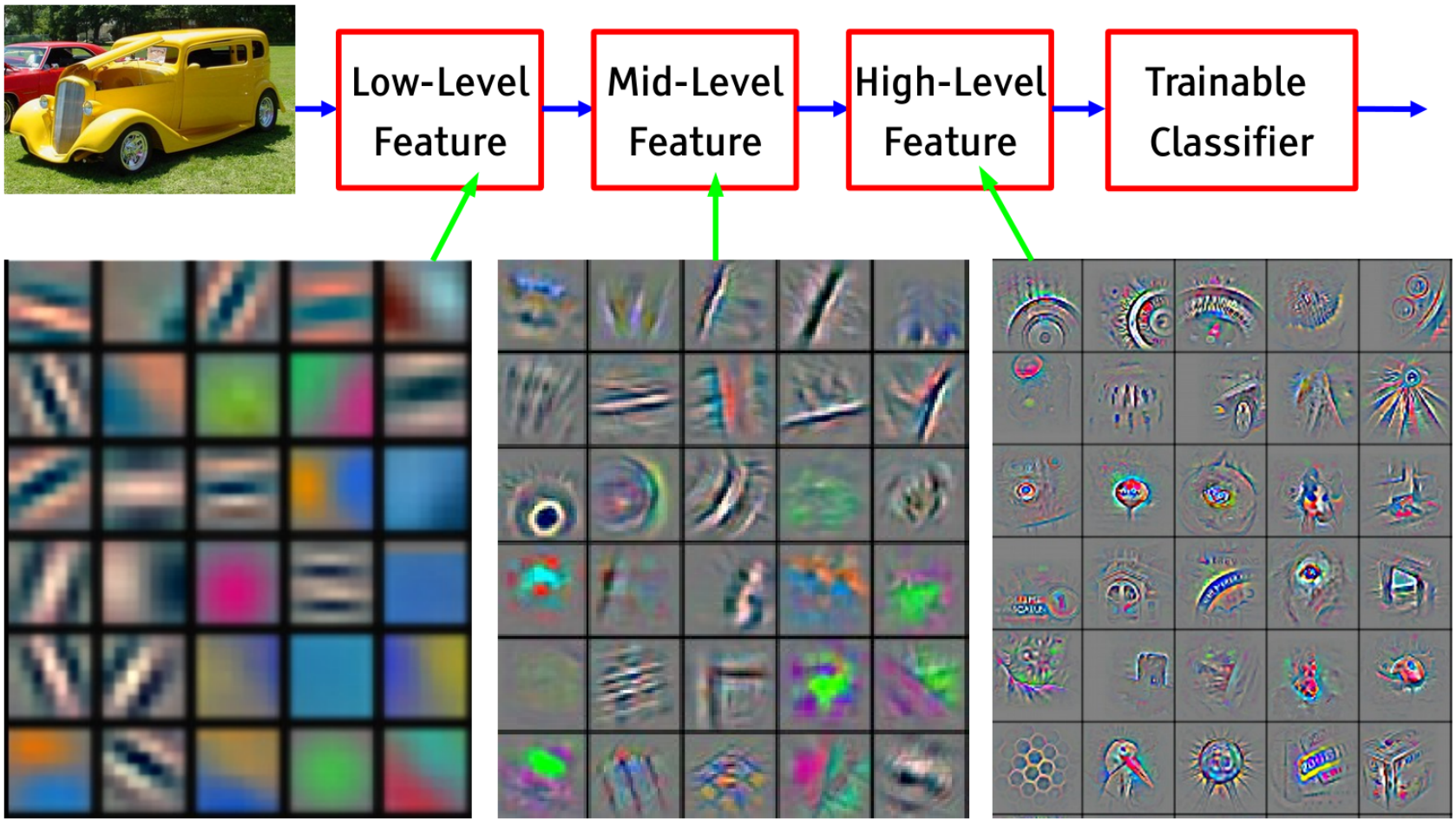


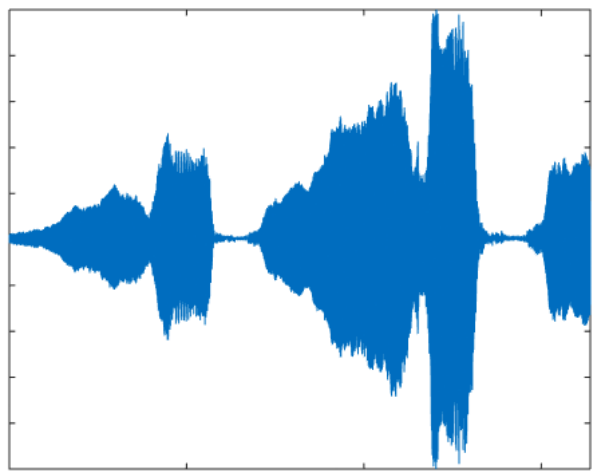
Figure: Features extracted from ImageNet.

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)

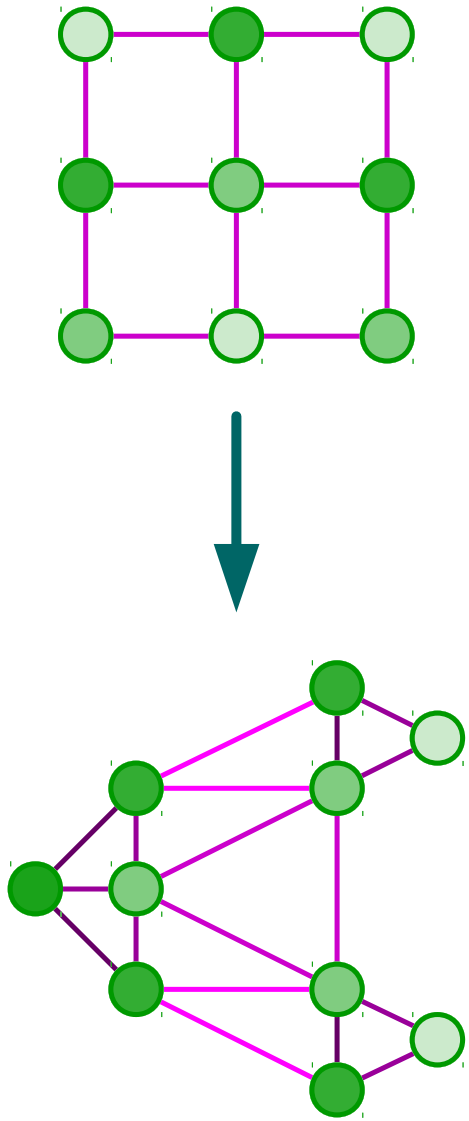


Sound (1D)

ConvNets on graphs

Graphs vs Euclidean grids

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



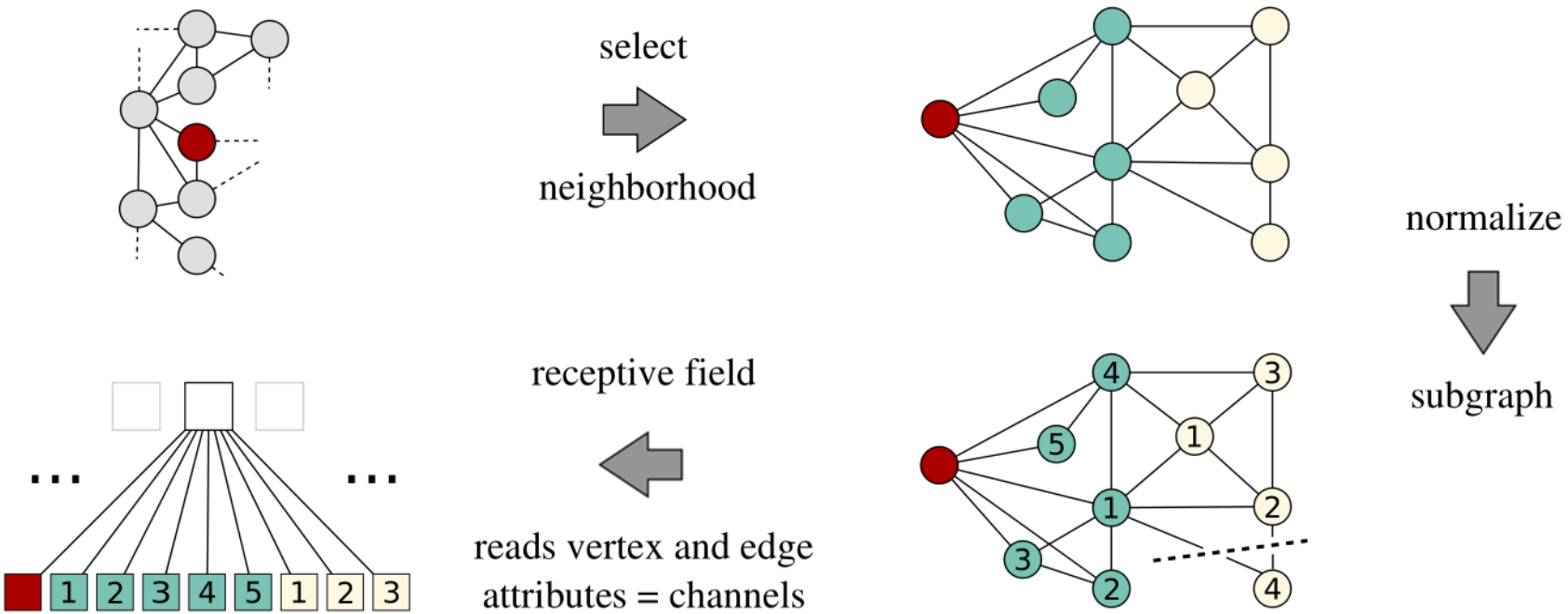
Challenges

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

ConvNets on graphs: spatial approach

Niepert, Ahmed, and Kutzkov 2016

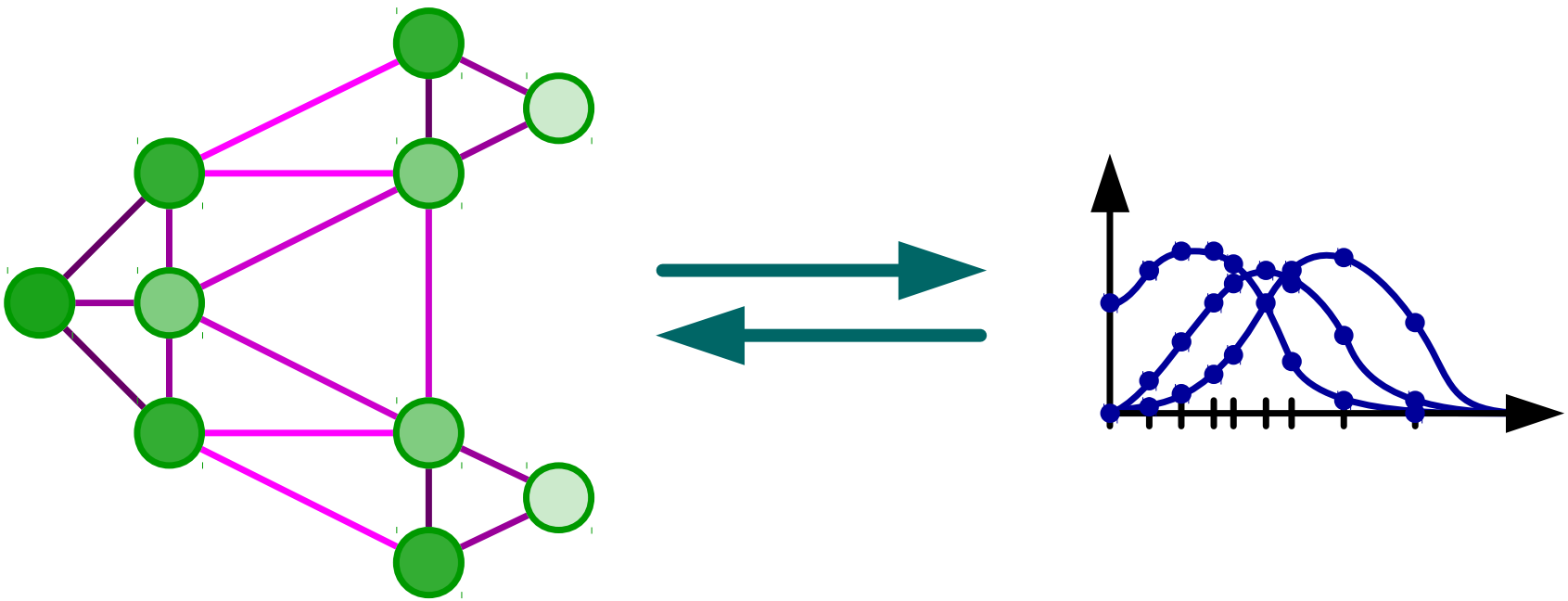
1. Define receptive field / neighborhood.
2. Order nodes, i.e. give an orientation.



ConvNets on graphs: spectral approach

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

- Spectral graph theory for convolution on graphs.
- Balanced cut model for graph coarsening (sub-sampling).

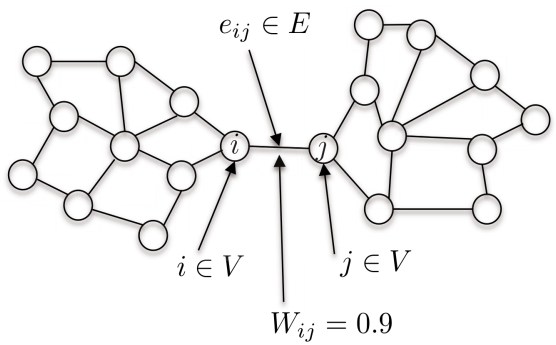


Definitions: graph

Chung 1997

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

G



- $\mathcal{V}$: 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

Definitions: graph Fourier transform

Shuman, Narang, Frossard, Ortega, and Vandergheynst 2013

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

- Graph Fourier basis $U = [u_0, \ldots, u_{n-1}] \in \mathbb{R}^{n \times n}$
- Graph "frequencies" $\Lambda = \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} \in \mathbb{R}^{n \times n}$

Graph Fourier Transform

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

Definitions: convolution on graphs

Shuman, Narang, Frossard, Ortega, and Vandergheynst 2013

Convolution theorem:

$$\begin{aligned} x *_{\mathcal{G}} g &= U\left(U^T g \odot U^T x\right) \\ &= U\left(\hat{g} \odot U^T x\right) \end{aligned}$$

Conveniently written as:

$$\begin{aligned} x *_{\mathcal{G}} g &= U \begin{bmatrix} \hat{g}(\lambda_1) & & 0 \\ & \ddots & \\ 0 & & \hat{g}(\lambda_n) \end{bmatrix} U^T x \\ &= U \hat{g}(\Lambda) U^T x \\ &= \hat{g}(L) x \end{aligned}$$

Spectral filtering of graph signals

$$y = \hat{g}_\theta(L)x = U\hat{g}_\theta(\Lambda)U^T x$$

Non-parametric filter:

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

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

Polynomial parametrization for localized filters

Shuman, Ricaud, and Vandergheynst 2016

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

- 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 $(L^K)_{i,j} = 0$
  (Hammond, Vandergheynst, and Gribonval 2011, Lemma 5.2)

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

Filter localization

Shuman, Ricaud, and Vandergheynst 2016

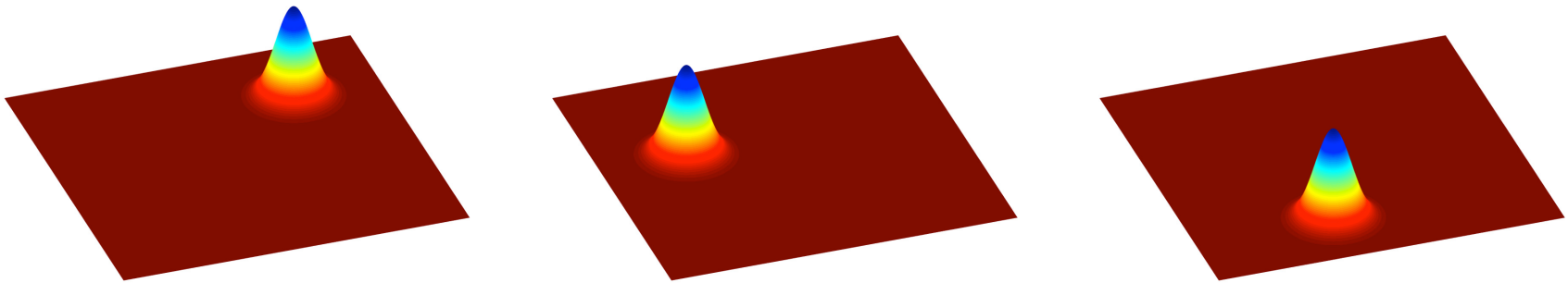


Figure: Localization on regular Euclidean grid.

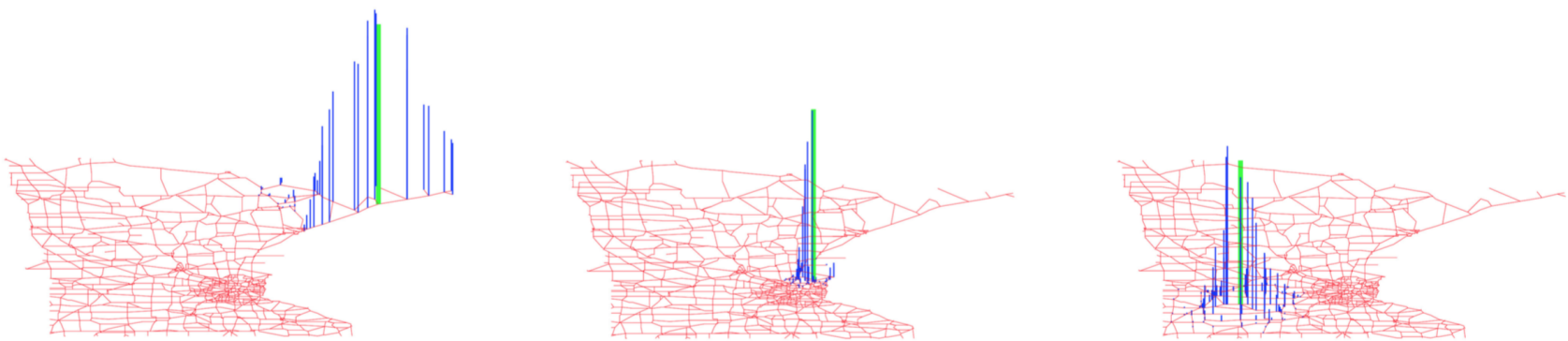


Figure: Localization on graph with $(\hat{g}_\theta(L)\delta_i)_j = (\hat{g}_\theta(L))_{i,j}$.

Recursive formulation for fast filtering

Hammond, Vandergheynst, and Gribonval 2011

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

- Chebyshev polynomials: $T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$ with $T_0 = 1$ and $T_1 = x$
- Filtering: $y = \hat{g}_\theta(L)x = \sum_{k=0}^{K-1} \theta_k T_k(\tilde{L})x$
- Recurrence: $y = \hat{g}_\theta(L)x = [\bar{x}_0, \ldots, \bar{x}_{K-1}]\theta$, $\bar{x}_k = T_k(\tilde{L})x = 2\tilde{L}\bar{x}_{k-1} - \bar{x}_{k-2}$ with $\bar{x}_0 = x$ and $\bar{x}_1 = \tilde{L}x$

- 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
  ($F_{in} \times F_{out}$ vectors of Chebyshev coefficients)

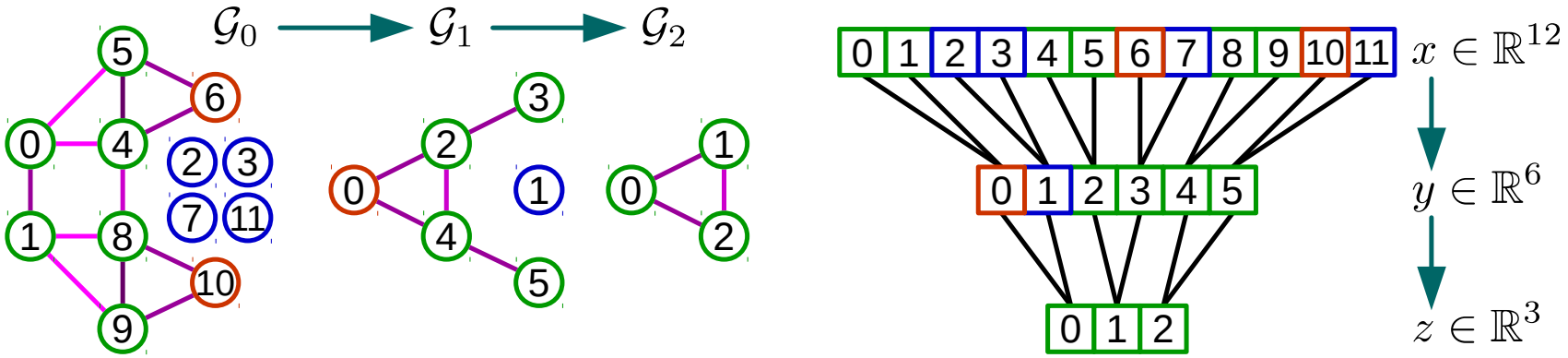
Gradients for backpropagation:

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

Overall cost of $\mathcal{O}(K|\mathcal{E}|F_{in}F_{out}S)$ operations

Coarsening & Pooling

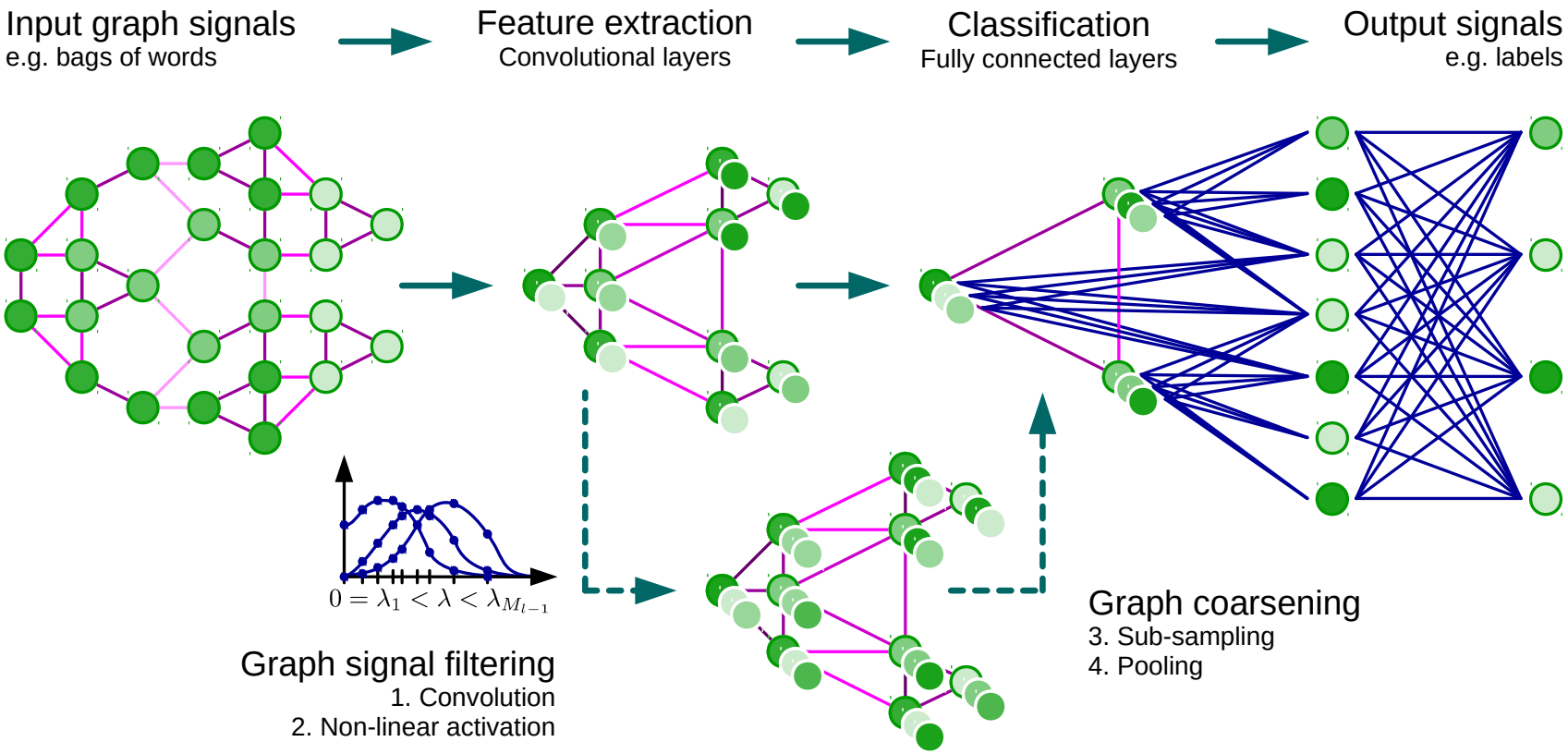
Defferrard, Bresson, and Vandergheynst 2016



- Coarsening: Graclus / Metis
  - Greedy node merging.
  - Very fast!
- Pooling: as regular 1D signals
  - Binary tree structured coarsened graphs.
  - Satisfies parallel architectures like GPUs.
- Activation: ReLU, LeakyReLU, maxout, tanh, sigmoid.

Graph ConvNet architecture

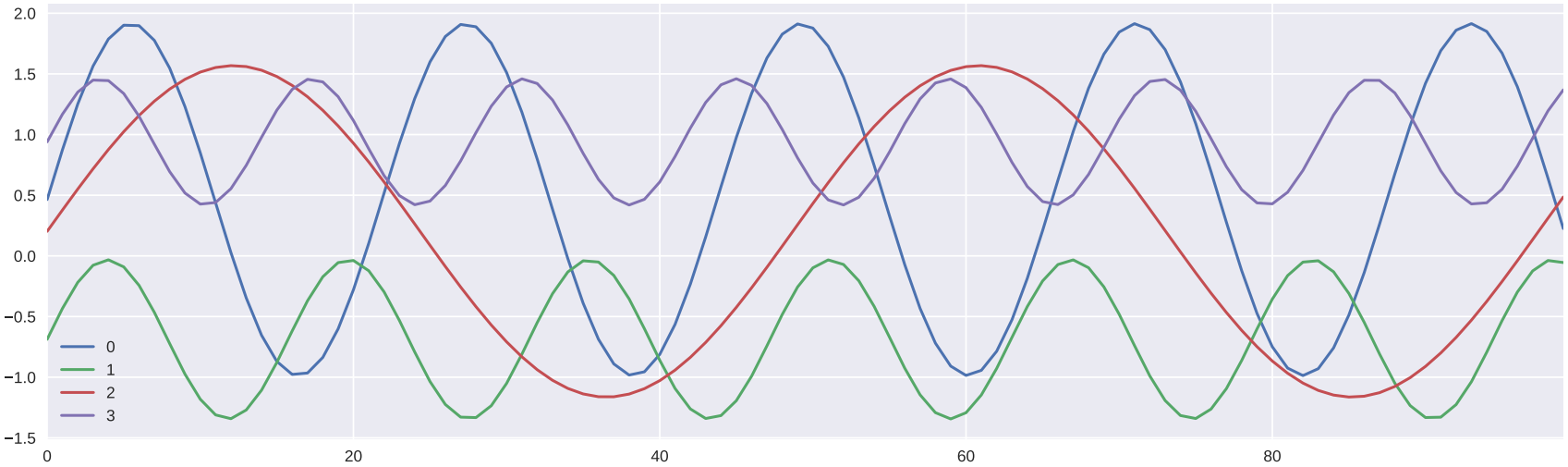
Defferrard, Bresson, and Vandergheynst 2016



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]

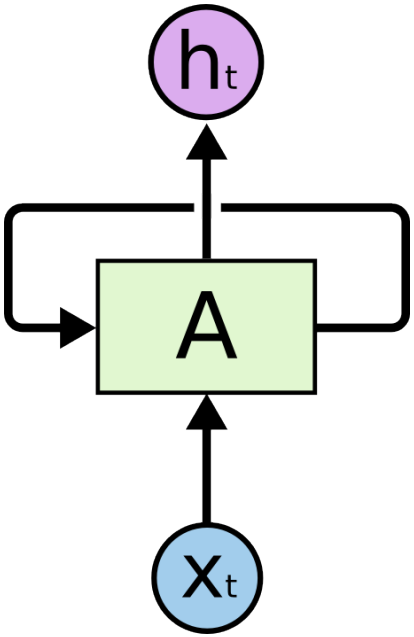
Time Series

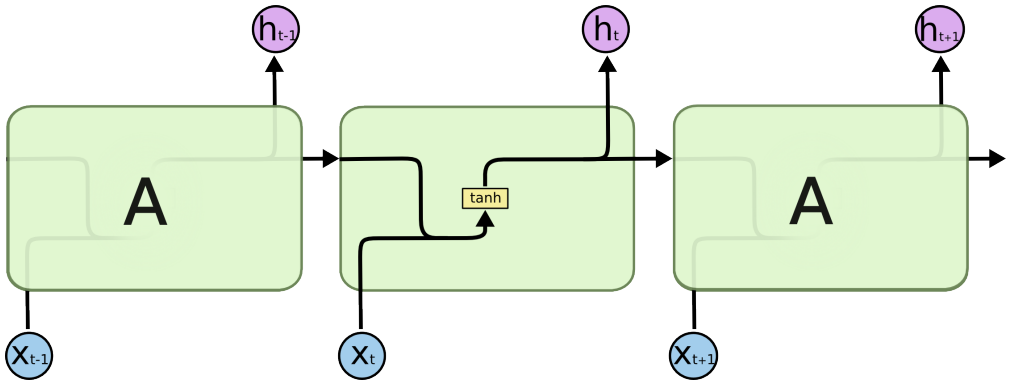


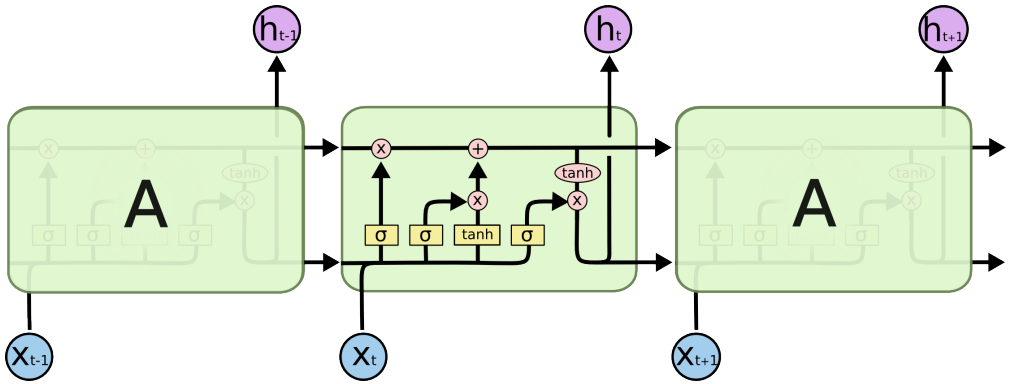
- Sensors: temperature, wind, pressure, body signals, etc.
- Stock market
- Text (series of discrete symbols, i.e. words)
- Network activity: energy, transportation, communication, brain

Recurrent Neural Networks & LSTM

Figures by Colah, 2015







Recurrent Graph Convolutional Network

Seo, Defferrard, Bresson, and Vandergheynst 2016

1D signals

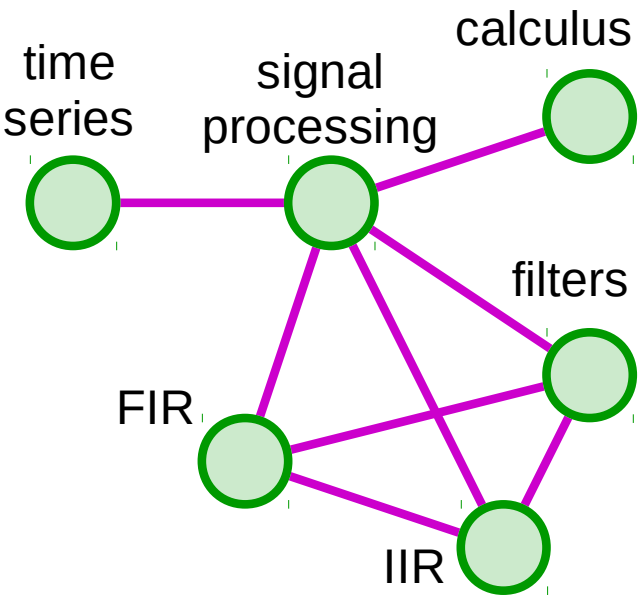
- $h_t = \tanh(W_x x_t + W_h h_{t-1})$
- $y_t = W h_t$
- State stored in hidden units

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.

Real data: Wikipedia

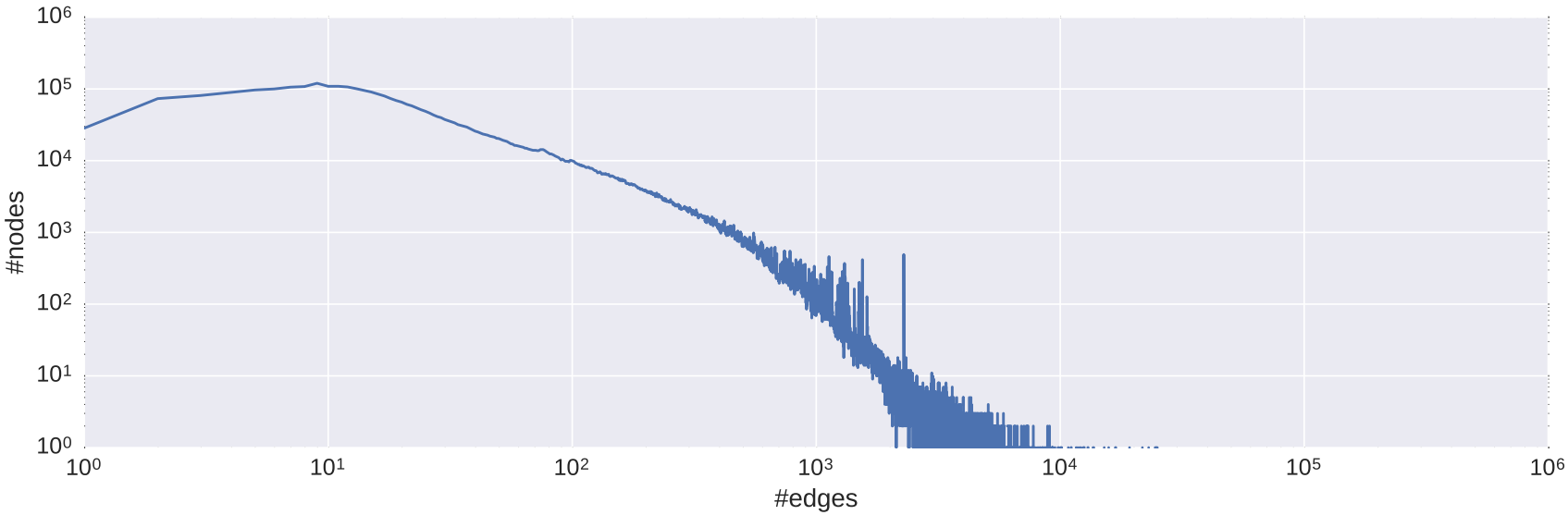


Goal: structured times series forecasting

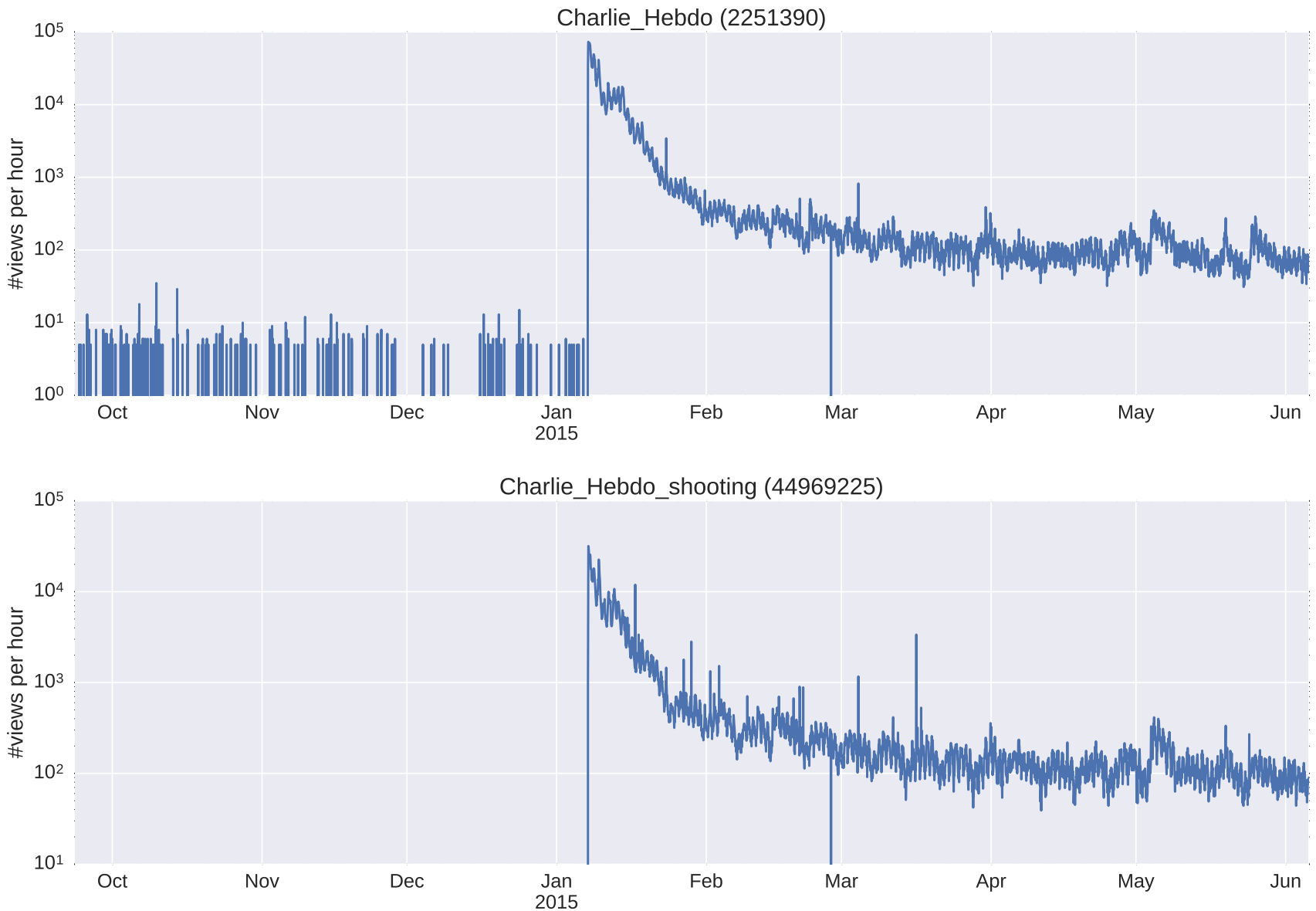
- Anomaly / event detection
- Regulation & Control
- Generative process understanding

Wikipedia network & signals

- Nodes: articles
- Edges: hyper-links
- Signals: number of hits per hour



Structured Time Series



Real data: Wikipedia

Real data (english wikipedia) is massive and hard

- 4.9M nodes
- 294M edges
- 6k time samples
- 760 GiB raw data
- dynamic: edges and nodes are added and removed

Example pruning: nodes with mean activity higher than 100 per hour

- 10k nodes
- 560k edges
- 6k time samples
- static: assume last hyper-link graph

Conclusion

- Graph are versatile tools to structure real data.
- Neural networks are the most effective ML algorithm today.

Deep Learning is coming to Graph Signal Processing

Further research

- Transfer between graphs / dynamic graphs
- Combine time & vertex domains with a joint transform
- Multi-scale approaches: both in time and vertex

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

Thanks Questions?

PS: next year, we're organizing the GSP workshop at EPFL!