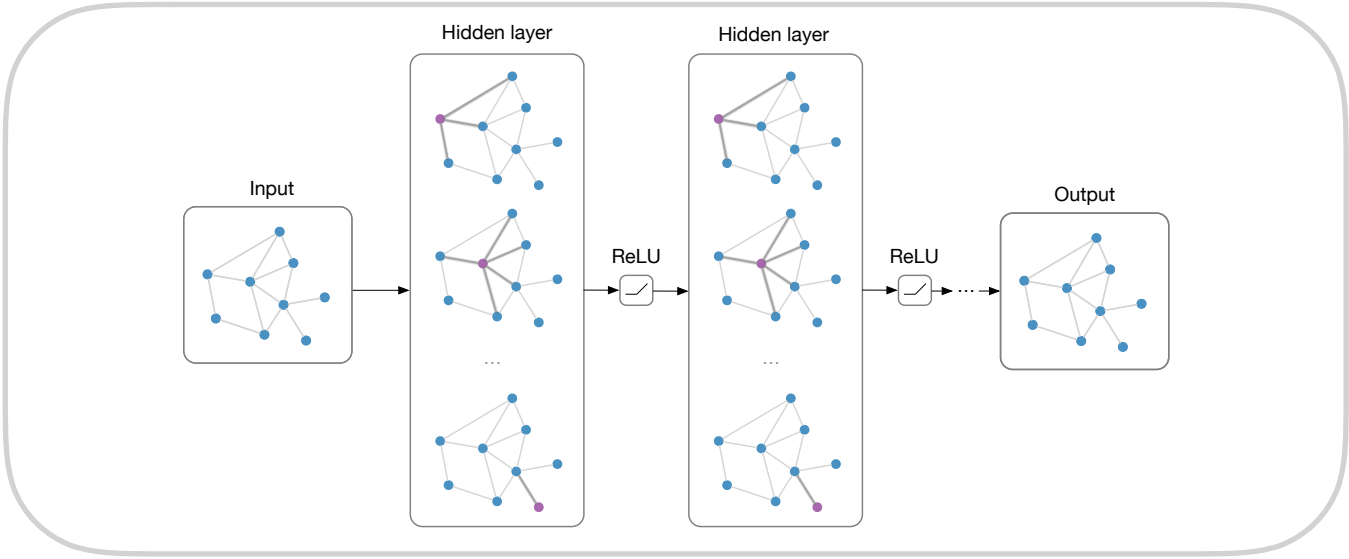
Deep Learning on Graphs with Graph Convolutional Networks



Thomas Kipf, 22 March 2017

joint work with Max Welling (University of Amsterdam)

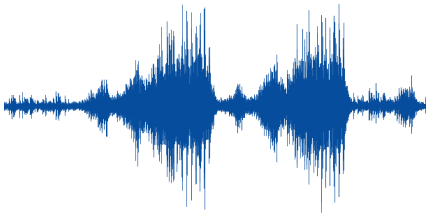
UNIVERSITEIT VAN AMSTERDAM

BDL Workshop @ NIPS 2016
Conference paper @ ICLR 2017
(+ new paper on arXiv)

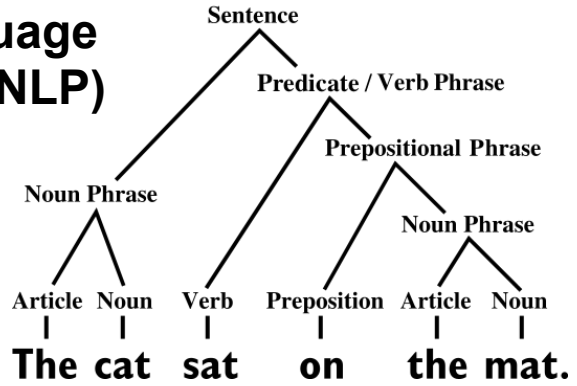
The success story of deep learning

IMAGENET

Speech data



Natural language processing (NLP)



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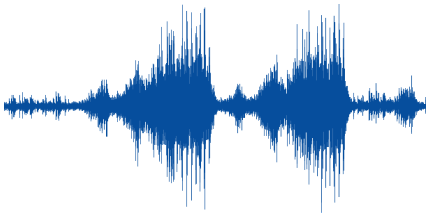

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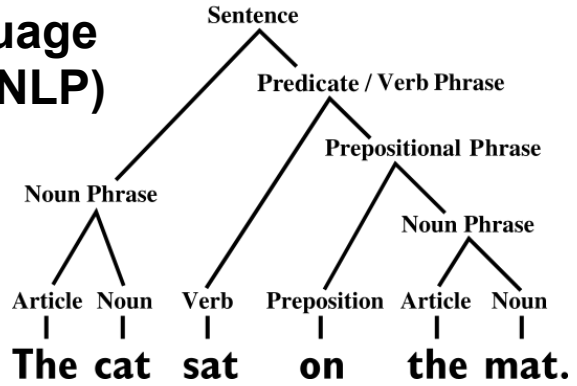
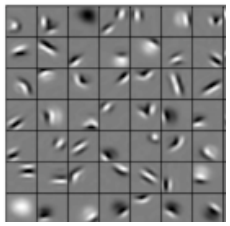
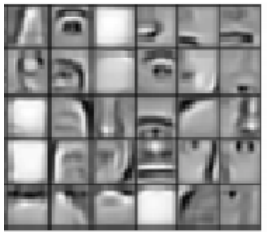


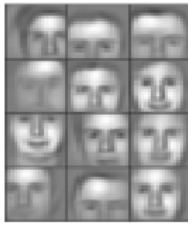
...

Deep neural nets that exploit:

- translation invariance (weight sharing)
- hierarchical compositionality

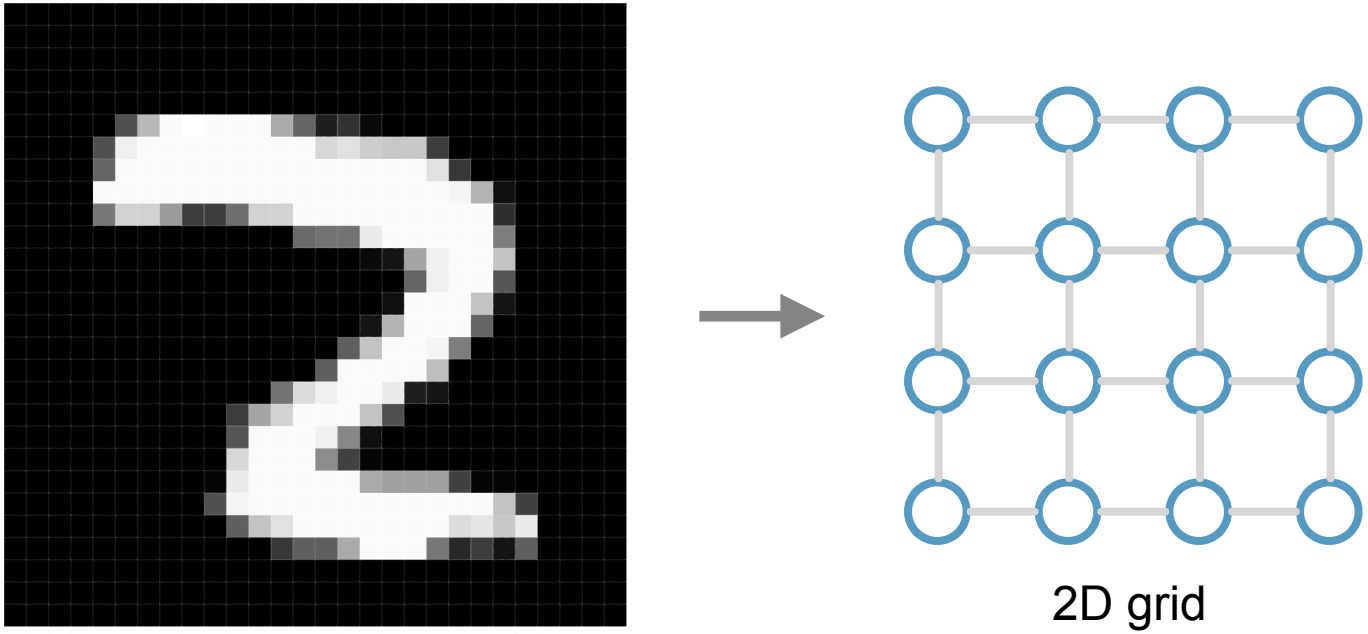






Recap: Deep learning on Euclidean data

Euclidean data: grids, sequences…



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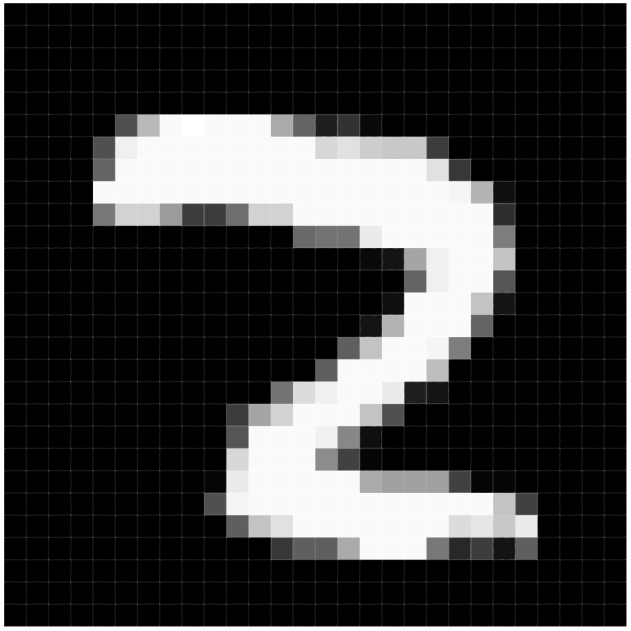
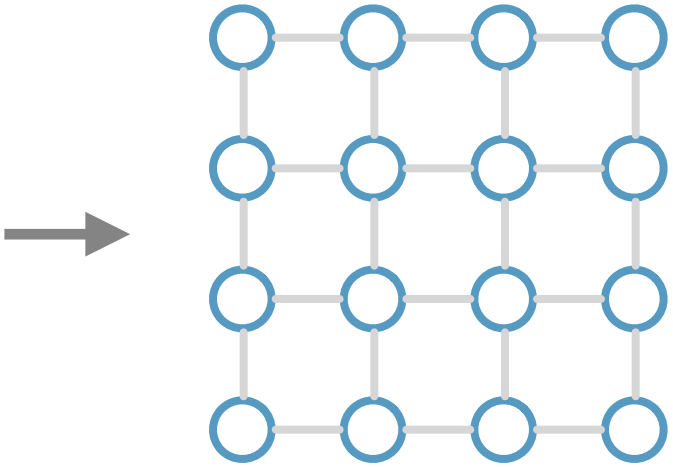
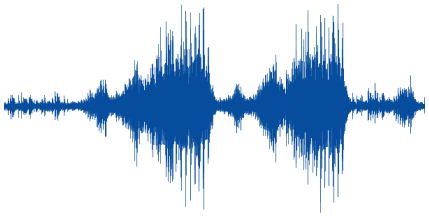




2D grid



1D grid

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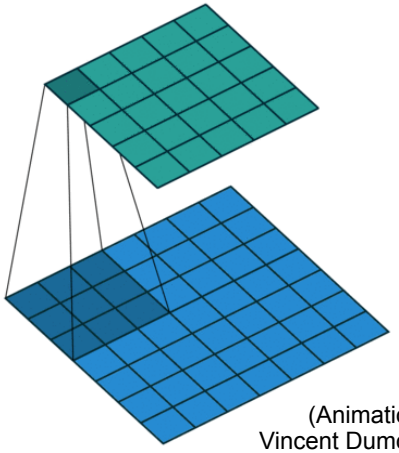
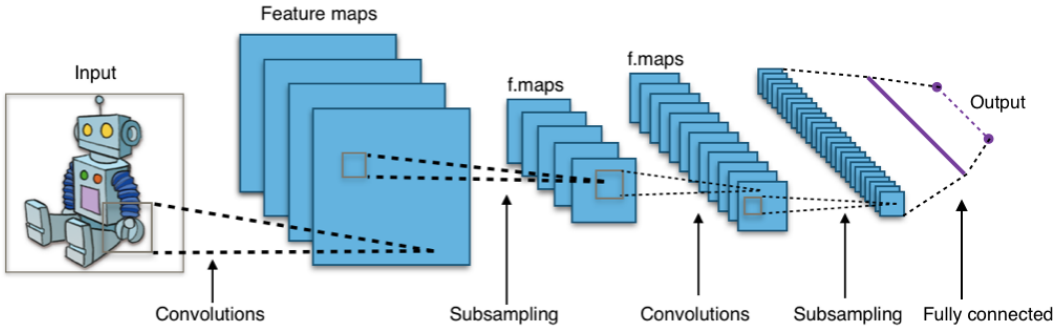
We know how to deal with this:

Convolutional neural networks (CNNs)



(Animation by Vincent Dumoulin)



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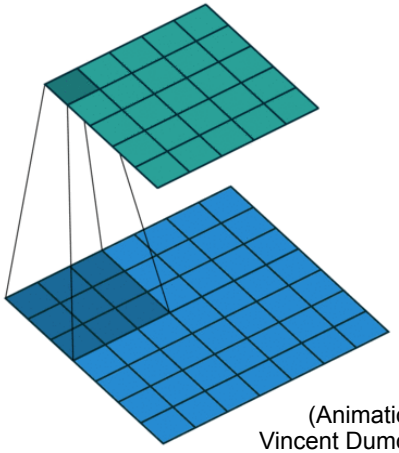

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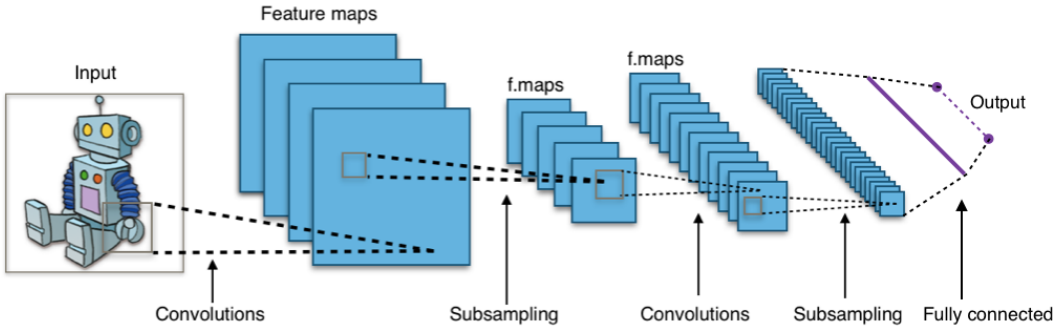

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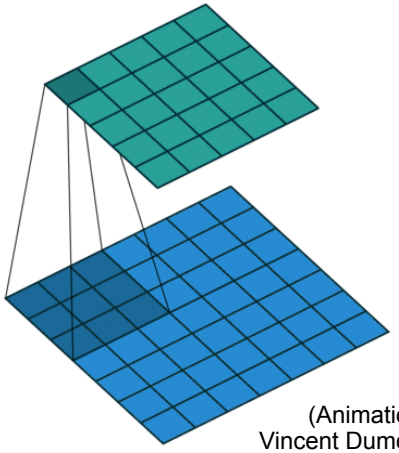

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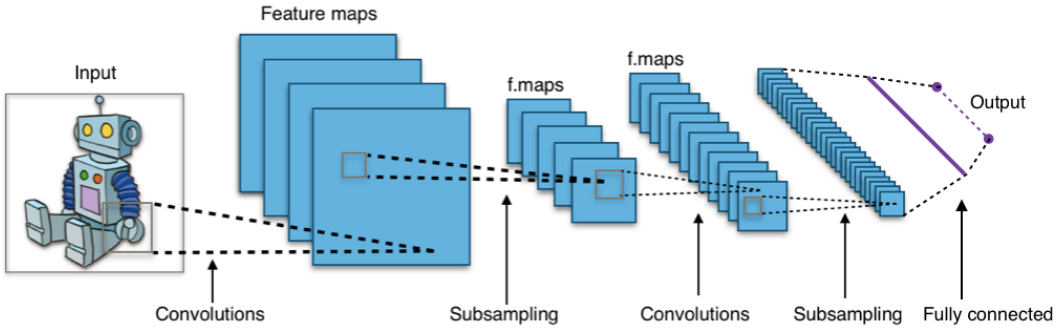
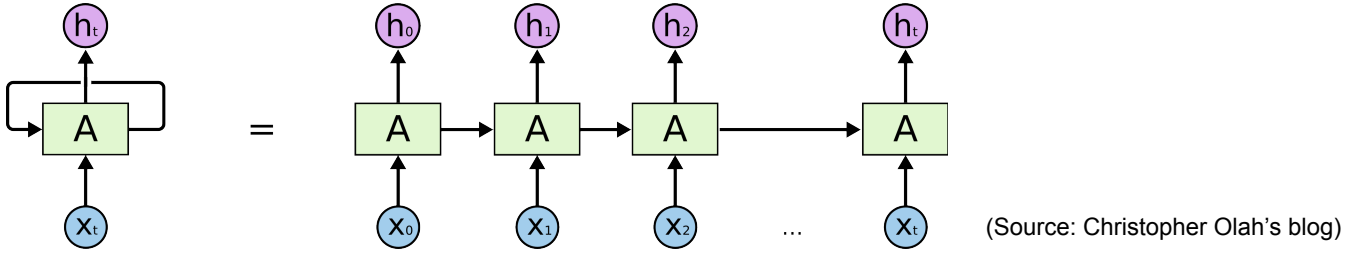


(Source: Wikipedia)

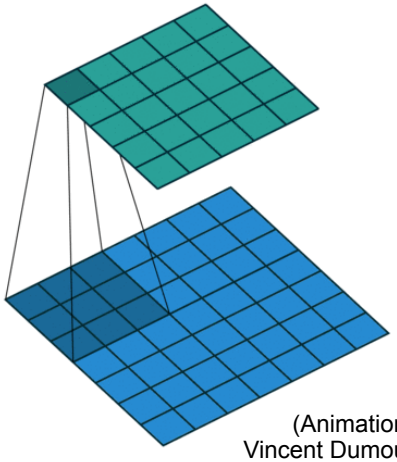
or recurrent neural networks (RNNs)



(Source: Christopher Olah's blog)

Convolutional neural networks (on grids)

Single CNN layer with 3x3 filter:



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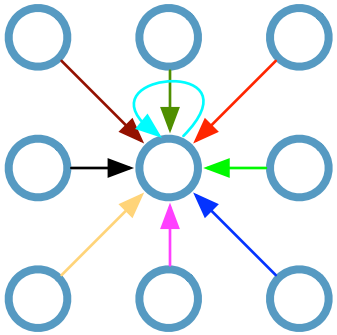

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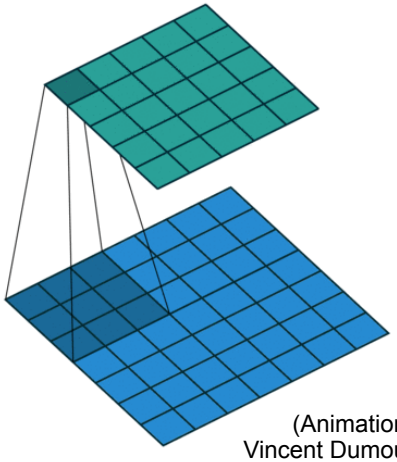

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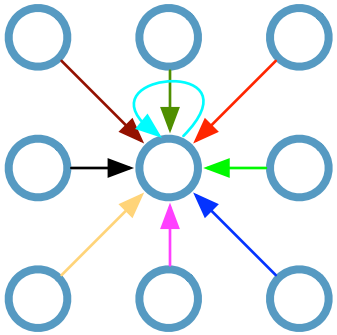

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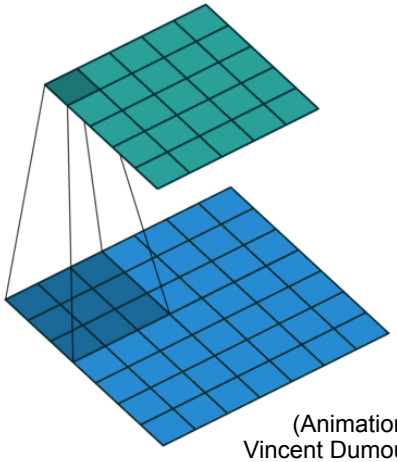

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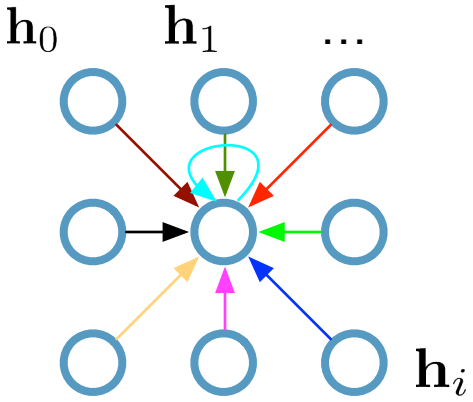

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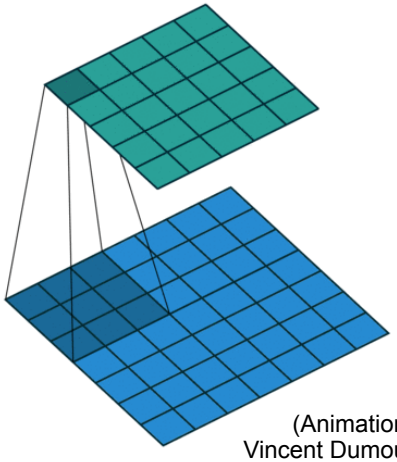

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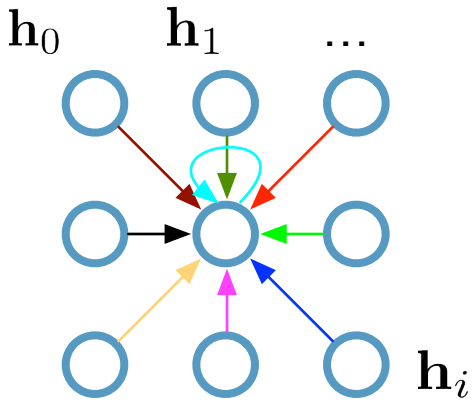

Update for a single pixel:

- Transform neighbors individually $\mathbf{W}_i \mathbf{h}_i$
- Add everything up $\sum_i \mathbf{W}_i \mathbf{h}_i$

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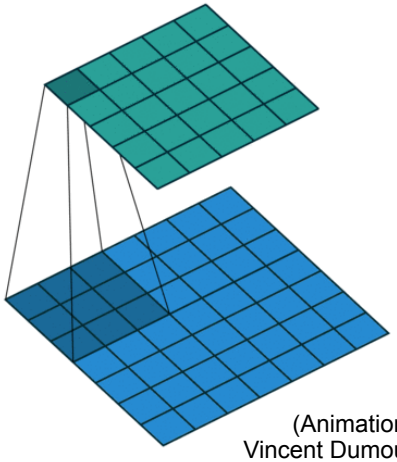

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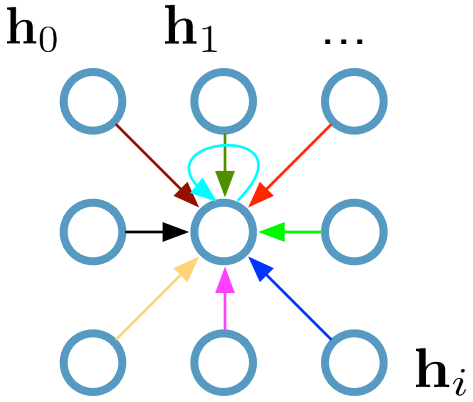

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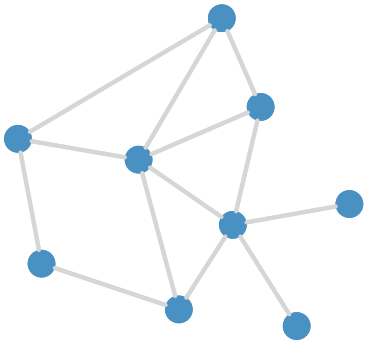
Full update: $\mathbf{h}_4^{(l+1)} = \sigma\left(\mathbf{W}_0^{(l)}\mathbf{h}_0^{(l)} + \mathbf{W}_1^{(l)}\mathbf{h}_1^{(l)} + \cdots + \mathbf{W}_8^{(l)}\mathbf{h}_8^{(l)}\right)$

Graph-structured data

What if our data looks like this?



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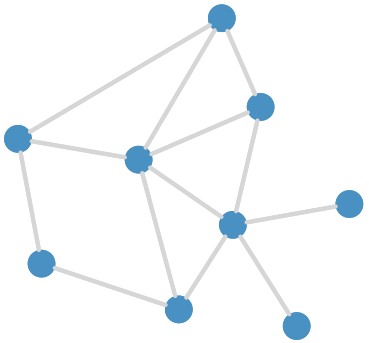

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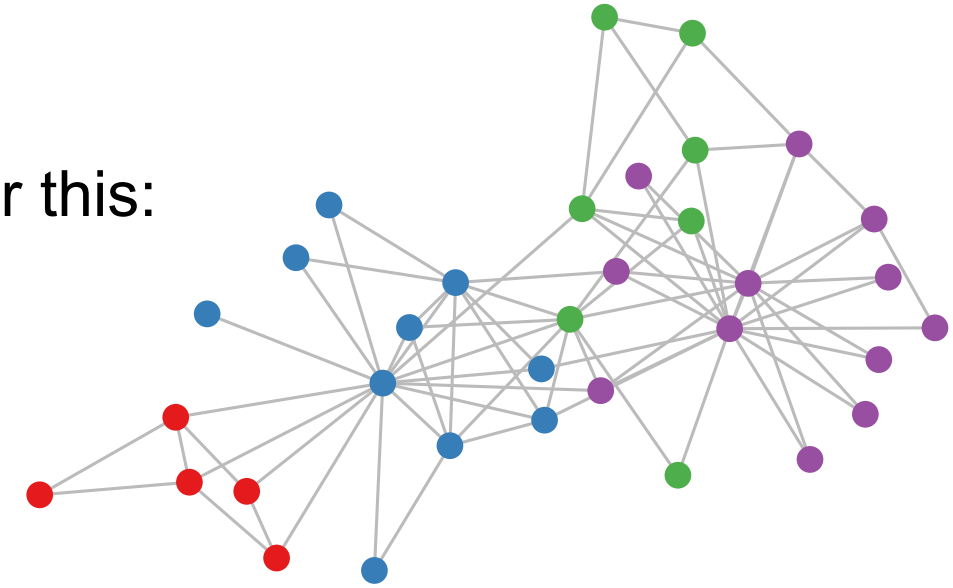

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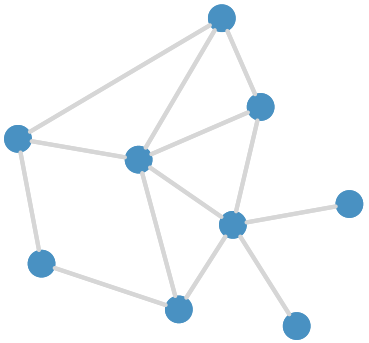

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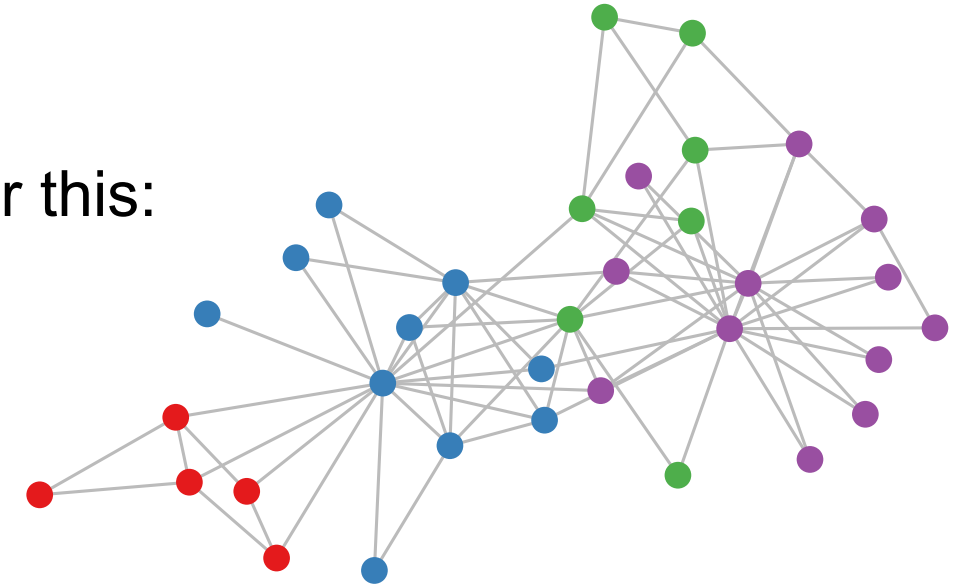


Real-world examples:

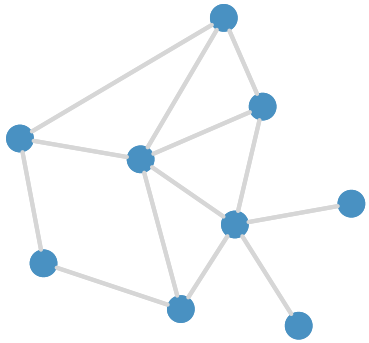
- Social networks
- World-wide-web
- Protein-interaction networks
- Telecommunication networks
- Knowledge graphs
- …

Graphs: Definitions

Graph: $G = (\mathcal{V}, \mathcal{E})$

$\mathcal{V}$: Set of nodes $\{v_i\}$, $|\mathcal{V}| = N$

$\mathcal{E}$: Set of edges $\{(v_i, v_j)\}$



We can define:

$\mathbf{A}$ (adjacency matrix): $A_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \in \mathcal{E} \\ 0 & \text{otherwise} \end{cases}$

(can also be weighted)

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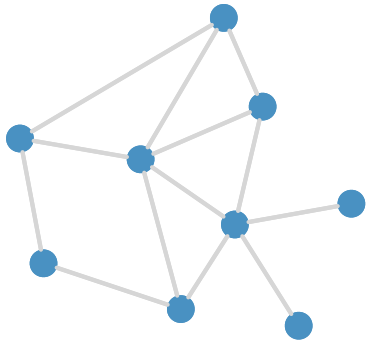

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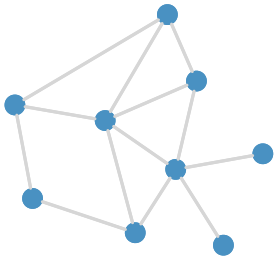
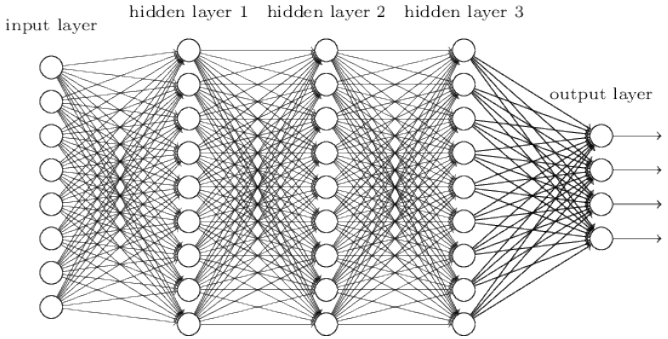
Model wish list:

- Set of trainable parameters $\{\mathbf{W}^{(l)}\}$
- Trainable in $\mathcal{O}(|\mathcal{E}|)$ time
- Applicable even if the input graph changes

A naive approach

- Take adjacency matrix $\mathbf{A}$ and feature matrix $\mathbf{X} \in \mathbb{R}^{N \times E}$
- Concatenate them $\mathbf{X}_{\text{in}} = [\mathbf{X}, \mathbf{A}] \in \mathbb{R}^{N \times (N+E)}$
- Feed them into deep (fully connected) neural net
- Done?





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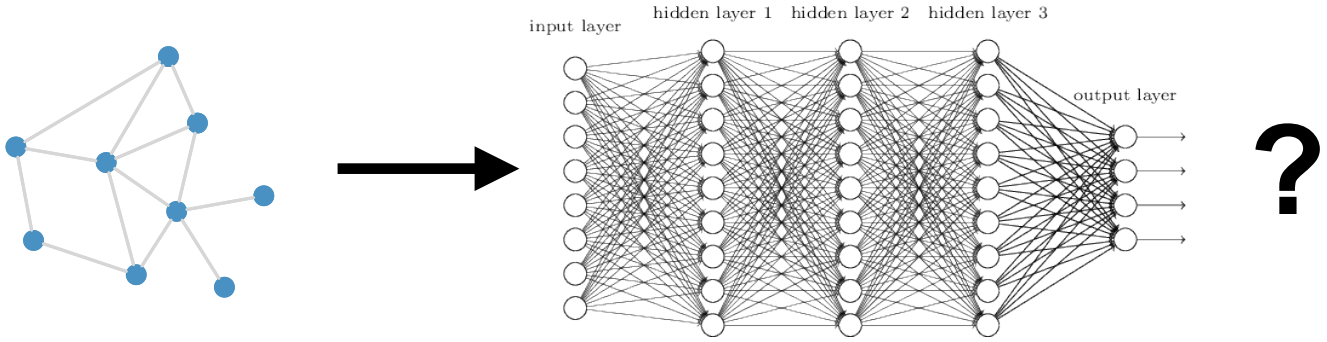

Problems:

- Huge number of parameters $\mathcal{O}(N)$
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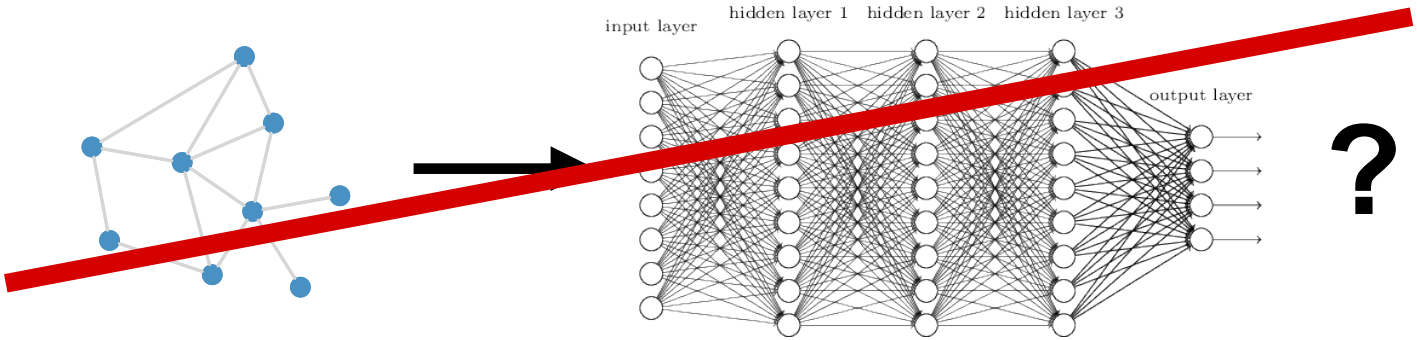

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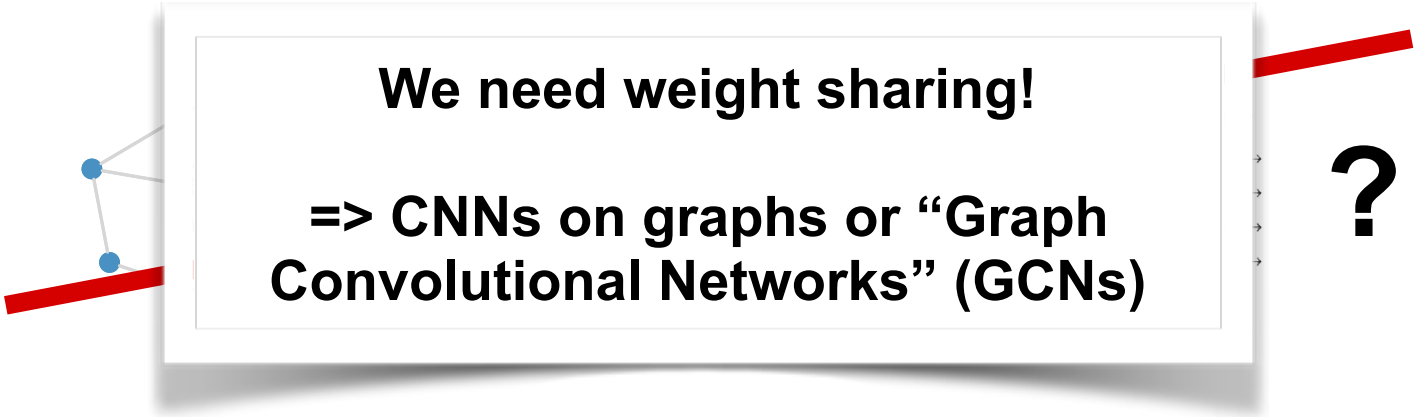

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CNNs on graphs with spatial filters

(related idea was first proposed in Scarselli et al. 2009)

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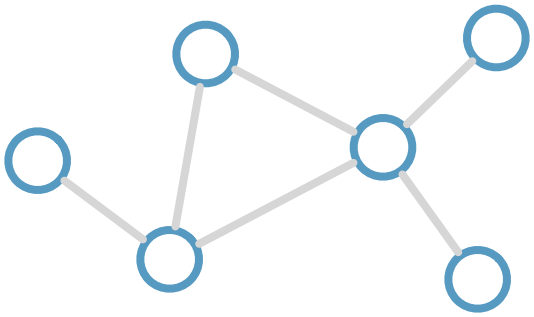

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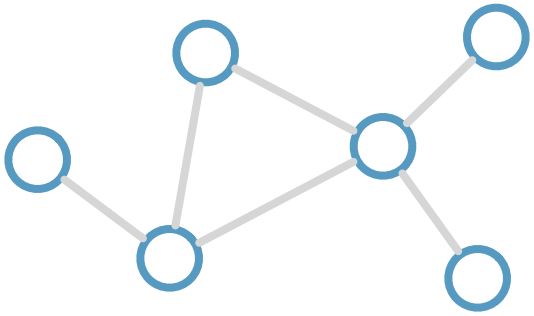

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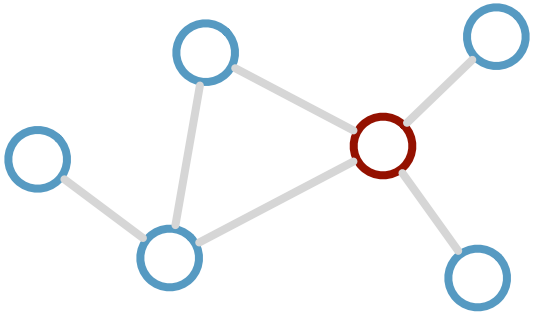

CNNs on graphs with spatial filters

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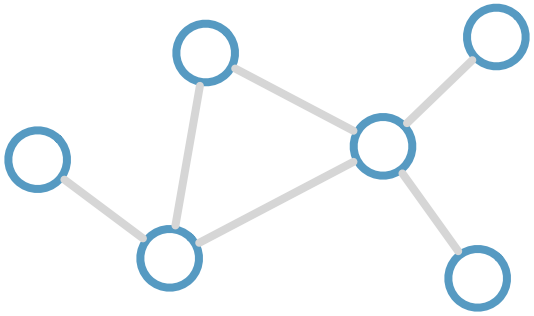

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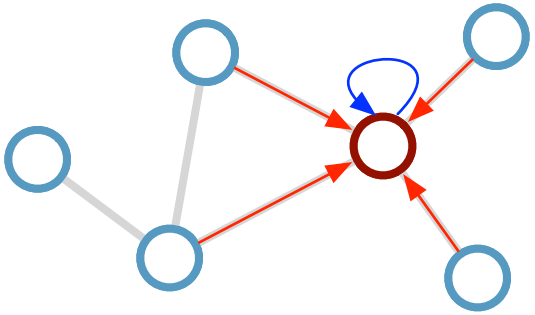

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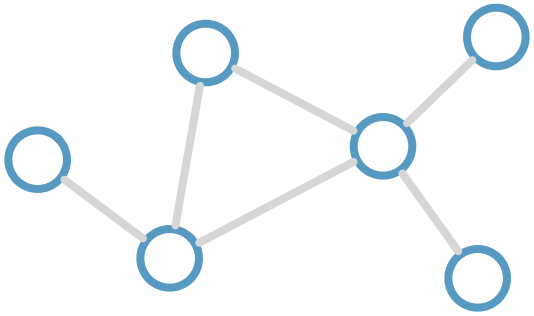

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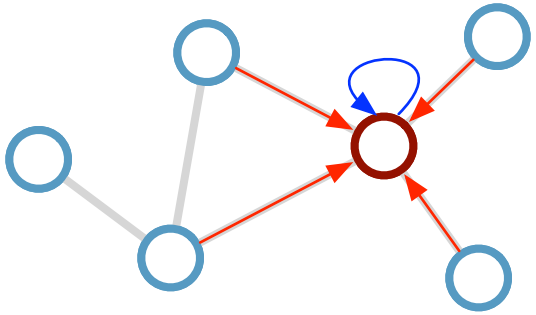

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$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j \in \mathcal{N}_i} \frac{1}{c_{ij}} \mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

$\mathcal{N}_i$: neighbor indices

c_{ij} : norm. constant (per edge)

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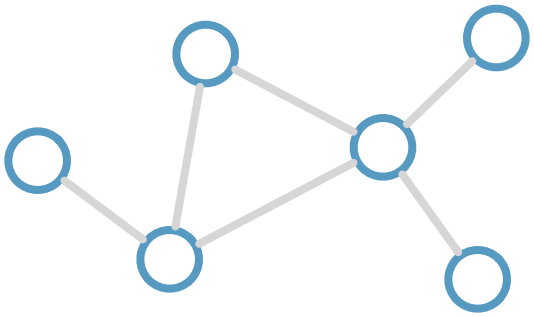

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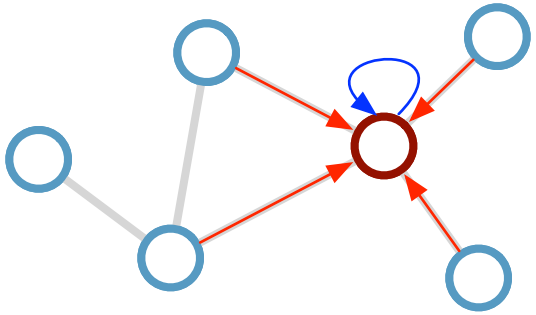

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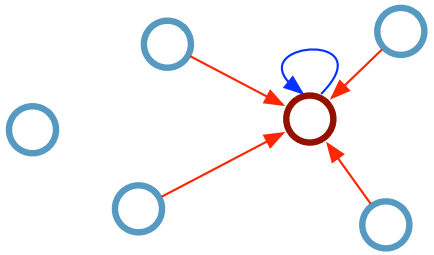
How is this related to spectral CNNs on graphs?

➡ Localized 1st-order approximation of spectral filters [Kipf & Welling, ICLR 2017]

Vectorized form

$$\mathbf{H}^{(l+1)} = \sigma\left(\mathbf{H}^{(l)}\mathbf{W}_0^{(l)} + \tilde{\mathbf{A}}\mathbf{H}^{(l)}\mathbf{W}_1^{(l)}\right)$$

with $\tilde{\mathbf{A}} = \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}$



$\mathbf{H}^{(l)} = [\mathbf{h}_1^{(l)^T}, \ldots, \mathbf{h}_N^{(l)^T}]^T$

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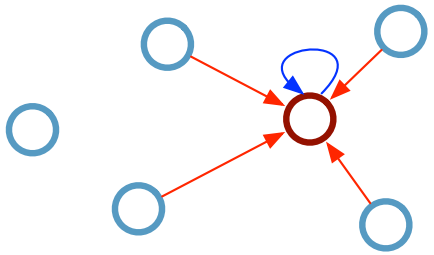

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Or treat self-connection in the same way:

$$\mathbf{H}^{(l+1)} = \sigma\left(\hat{\mathbf{A}}\mathbf{H}^{(l)}\mathbf{W}_1^{(l)}\right)$$

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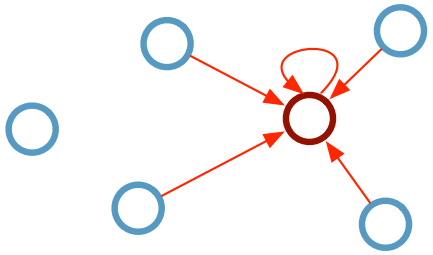

$\tilde{D}_{ii} = \sum_j (A_{ij} + \delta_{ij})$

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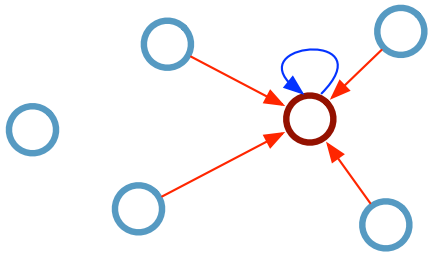

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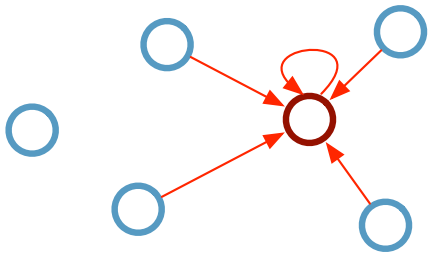

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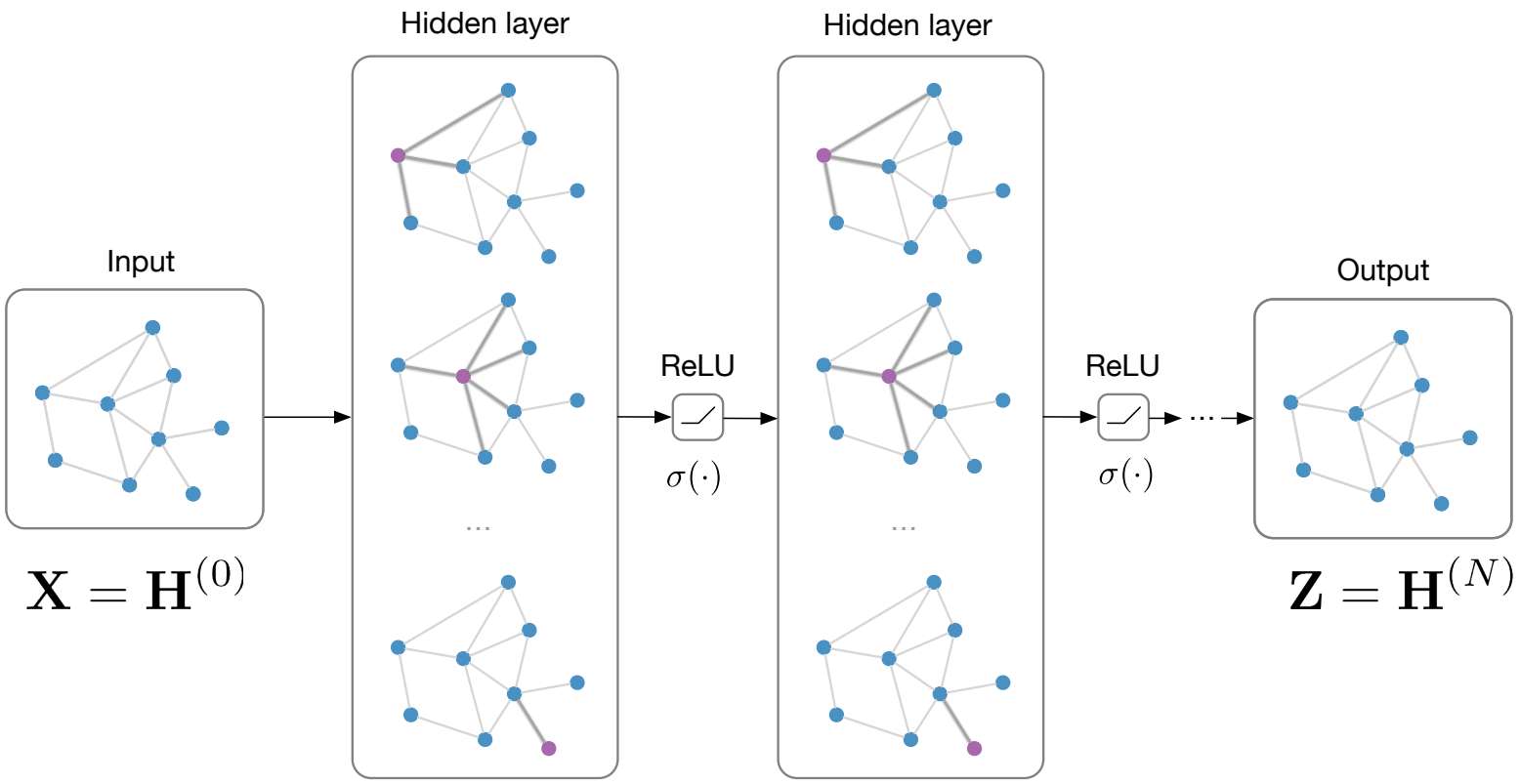
$\mathbf{A}$ is typically **sparse**

- ➡ We can use sparse matrix multiplications!
- ➡ Efficient $\mathcal{O}(|\mathcal{E}|)$ implementation in Theano or TensorFlow

Model architecture (with spatial filters)

Input: Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times E}$, preprocessed adjacency matrix $\hat{\mathbf{A}}$



$$\mathbf{H}^{(l+1)} = \sigma\left(\hat{\mathbf{A}}\mathbf{H}^{(l)}\mathbf{W}^{(l)}\right)$$

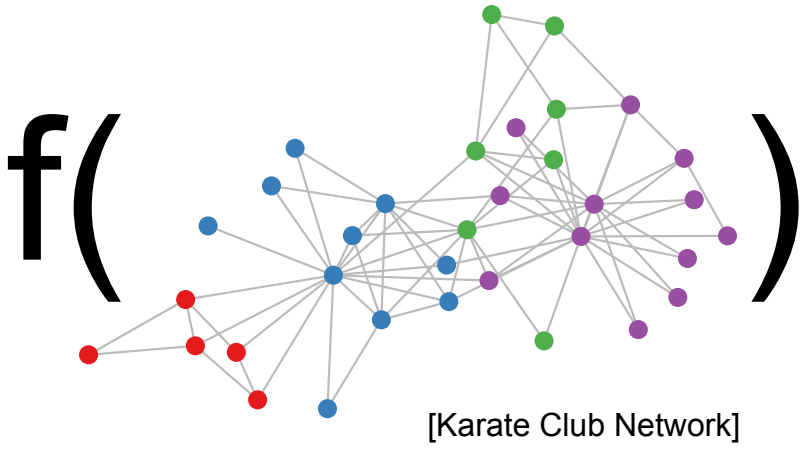
(or more sophisticated filters / basis functions)

[Kipf & Welling, ICLR 2017]

What does it do? An example.

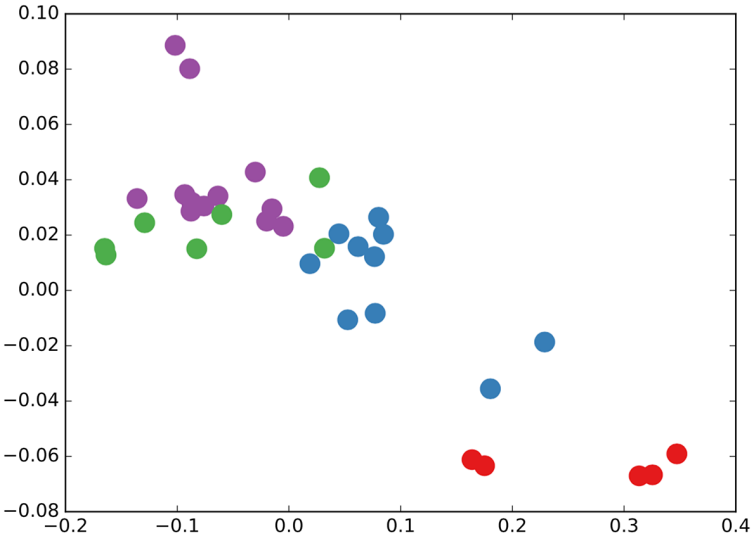
Forward pass through **untrained** 3-layer GCN model

Parameters initialized randomly



[Karate Club Network]

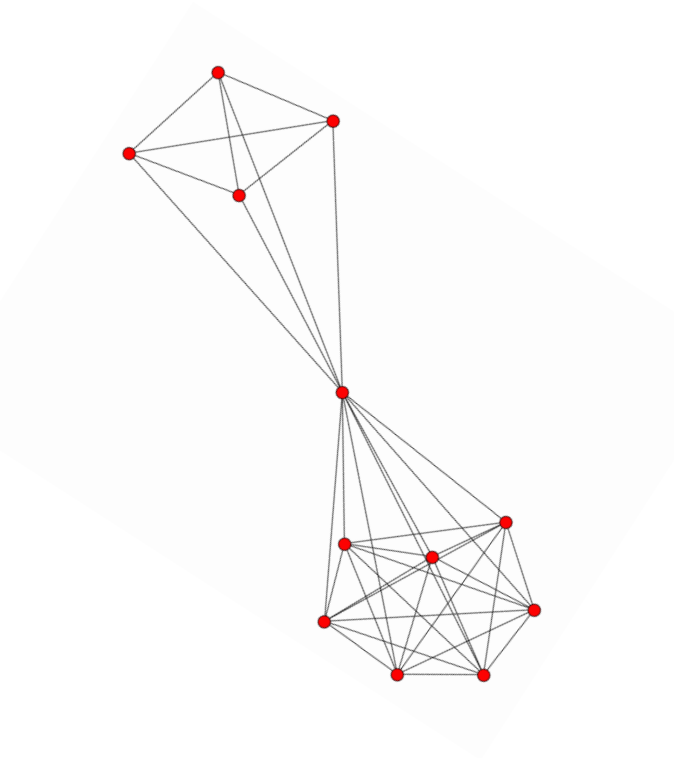
2-dim output per node



Produces (useful?) random embeddings!

Connection to Weisfeiler-Lehman algorithm

A “classical” approach for node feature assignment



Algorithm 1: WL-1 algorithm (Weisfeiler & Lehmann, 1968)

Input: Initial node coloring $(h_1^{(0)}, h_2^{(0)}, ..., h_N^{(0)})$

Output: Final node coloring $(h_1^{(T)}, h_2^{(T)}, ..., h_N^{(T)})$

$t \leftarrow 0$;

repeat

  for $v_i \in \mathcal{V}$ **do**

    $h_i^{(t+1)} \leftarrow \text{hash}\left(\sum_{j \in \mathcal{N}_i} h_j^{(t)}\right)$;

  $t \leftarrow t + 1$;

until *stable node coloring is reached*;

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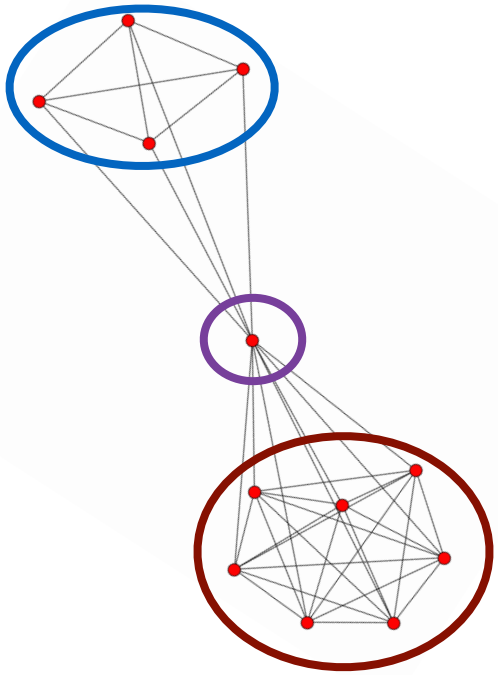

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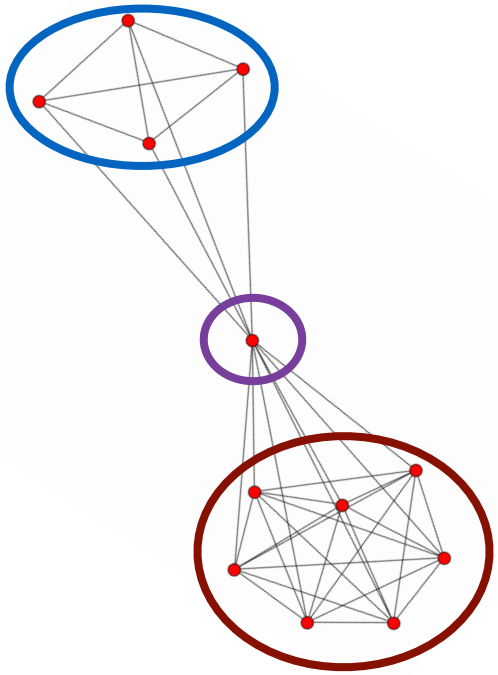

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Useful as graph isomorphism check for *most* graphs

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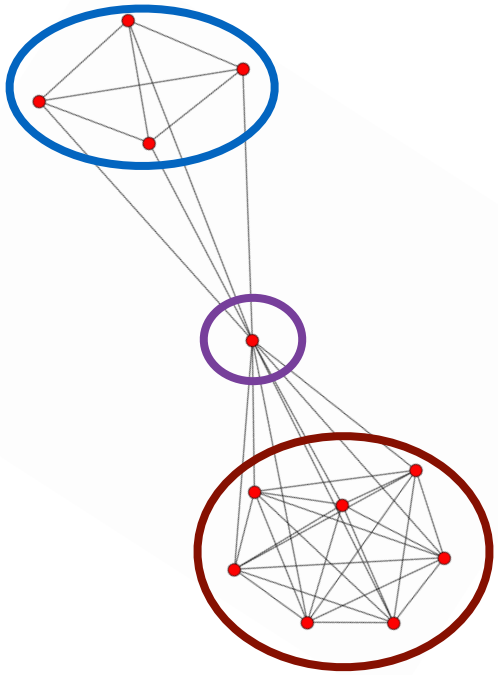

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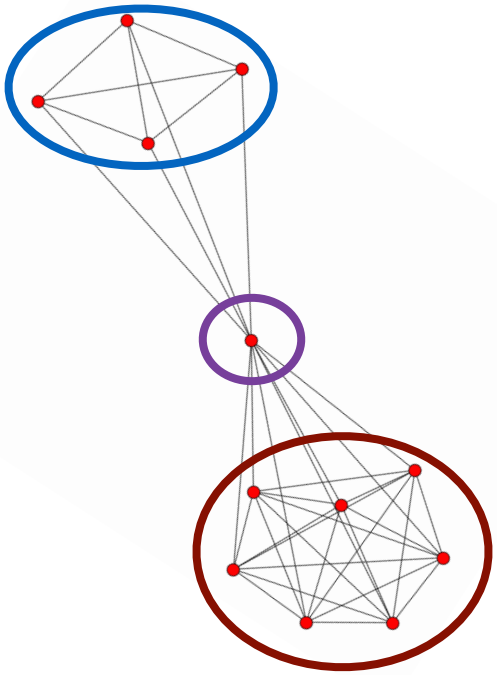

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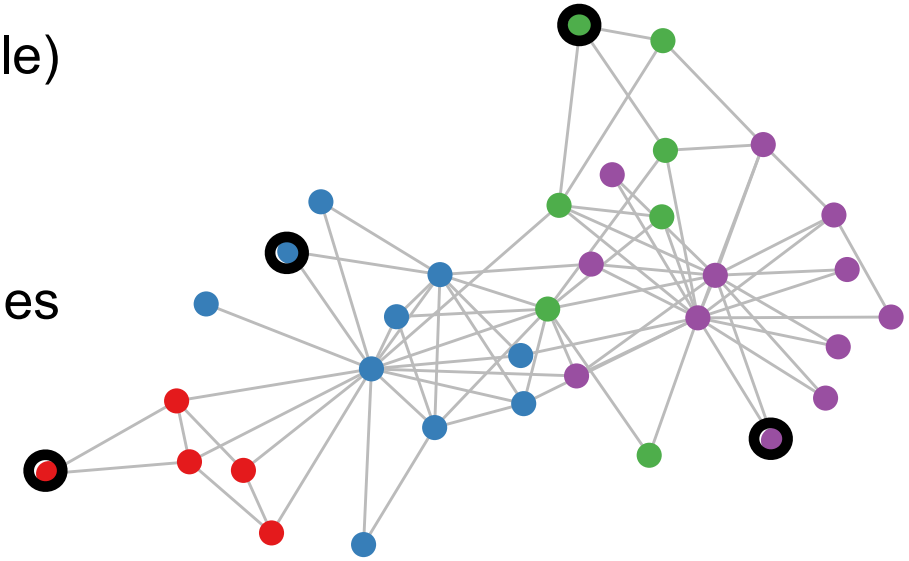
Semi-supervised classification on graphs

Setting:

Some nodes are labeled (black circle)
All other nodes are unlabeled

Task:

Predict node label of unlabeled nodes



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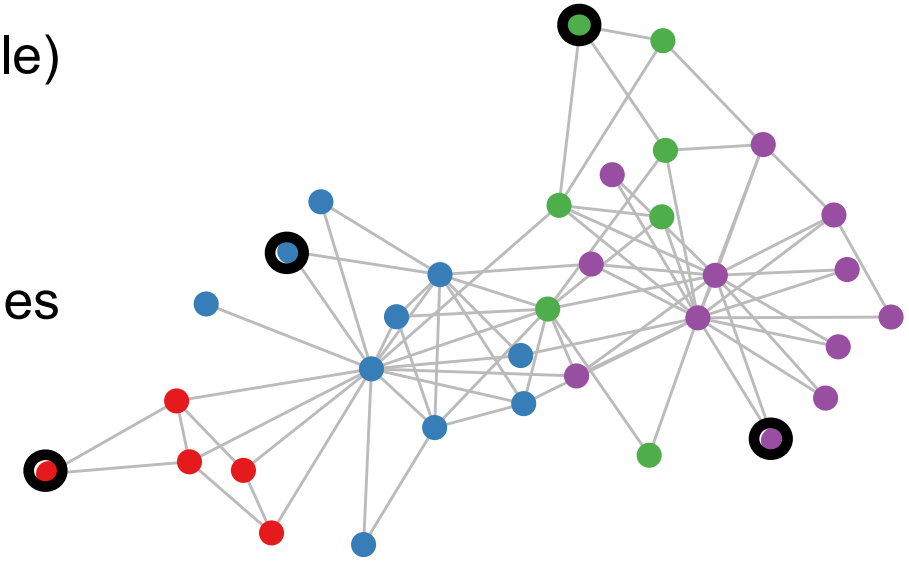

Task:

Predict node label of unlabeled nodes

Standard approach:

graph-based regularization ("smoothness constraints") [Zhu et al., 2003]

$$\mathcal{L} = \mathcal{L}_0 + \lambda \mathcal{L}_{\text{reg}} \quad \text{with} \quad \mathcal{L}_{\text{reg}} = \sum_{i,j} A_{ij} \| f(X_i) - f(X_j) \|^2$$

assumes: connected nodes likely to share same label

Semi-supervised classification on graphs

Embedding-based approaches

Two-step pipeline:

1) Get embedding for every node
2) Train classifier on node embedding

Examples: DeepWalk [Perozzi et al., 2014], node2vec [Grover & Leskovec, 2016]

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Problem: Embeddings are not optimized for classification!

Idea: Train graph-based classifier end-to-end using GCN

Evaluate loss on labeled nodes only:

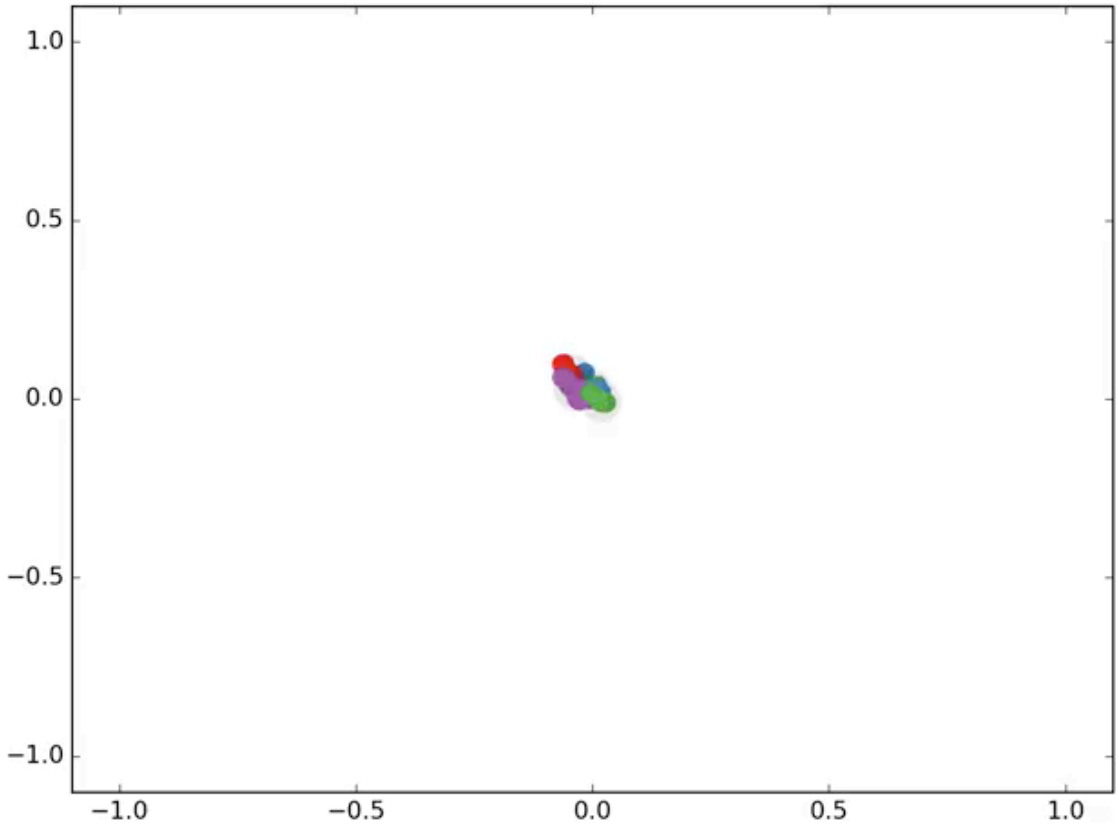
$$\mathcal{L} = - \sum_{l \in \mathcal{Y}_L} \sum_{f=1}^{F} Y_{lf} \ln Z_{lf}$$

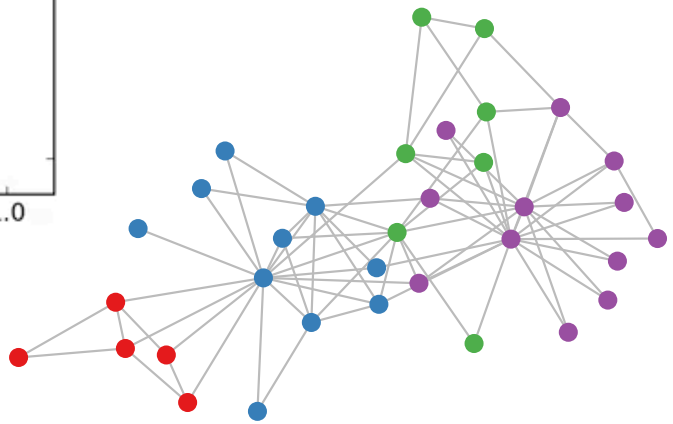
$\mathcal{Y}_L$ set of labeled node indices

$\mathbf{Y}$ label matrix

$\mathbf{Z}$ GCN output (after softmax)

Toy example (semi-supervised learning)





Video also available here:
http://tkipf.github.io/graph-convolutional-networks

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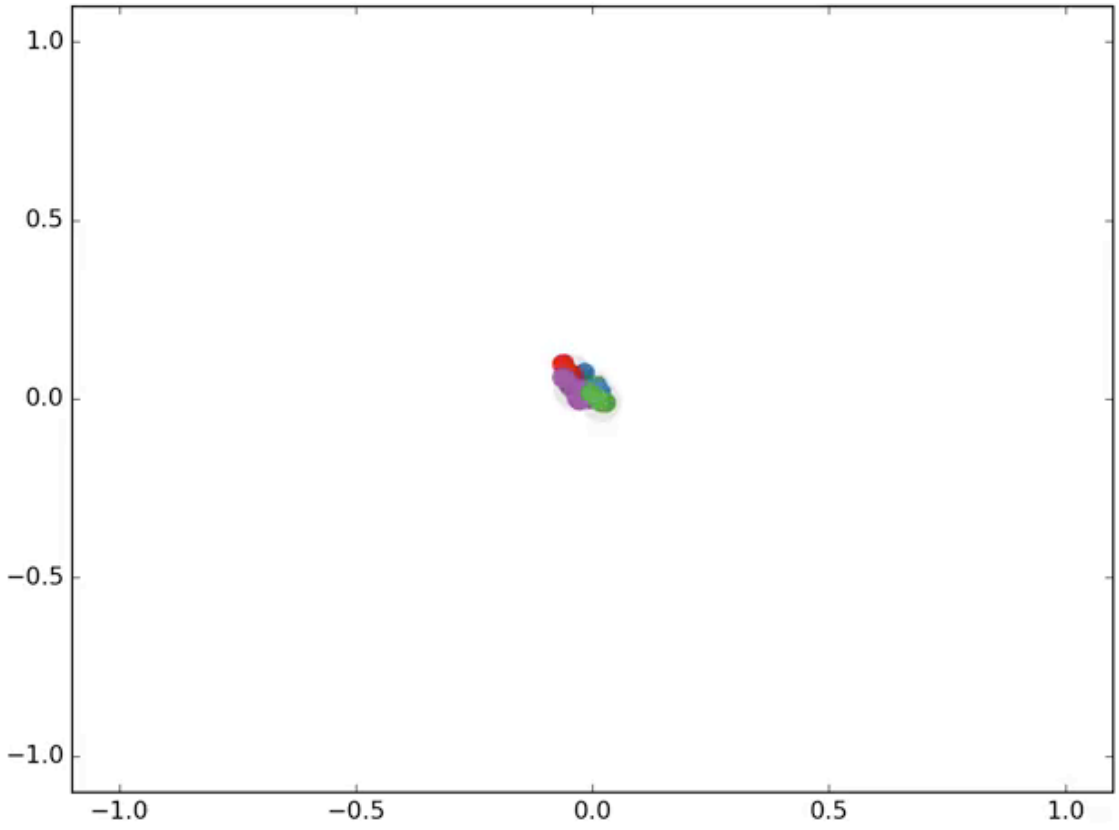

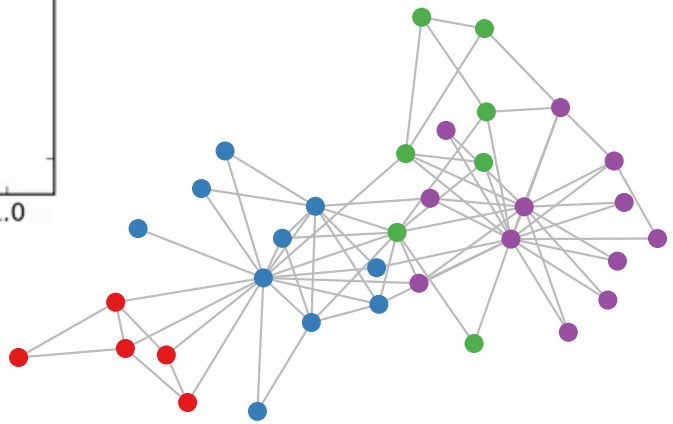

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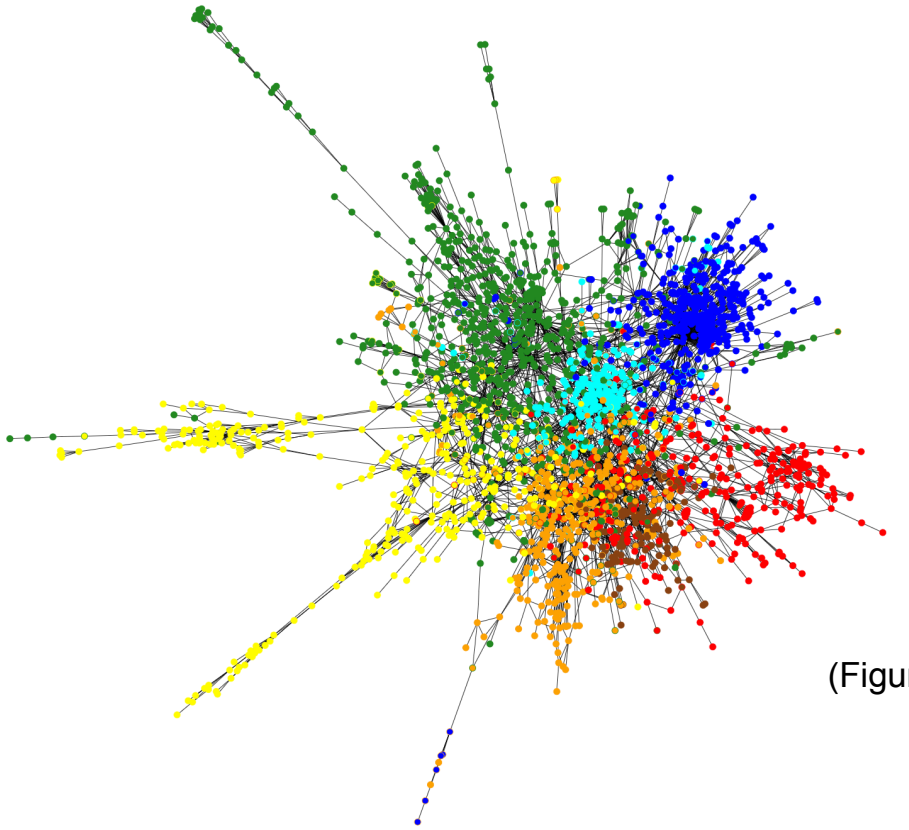
Classification on citation networks

Input: Citation networks (nodes are papers, edges are citation links, optionally bag-of-words features on nodes)

Target: Paper category (e.g. stat.ML, cs.LG, …)



(Figure from: Bronstein, Bruna, LeCun, Szlam, Vandergheynst, 2016)

Experiments and results

Model: 2-layer GCN $Z = f(X, A) = \mathrm{softmax}\Big(\hat{A}\ \mathrm{ReLU}\Big(\hat{A}XW^{(0)}\Big)\ W^{(1)}\Big)$

Dataset statistics

Dataset	Type	Nodes	Edges	Classes	Features	Label rate
Citeseer	Citation network	3,327	4,732	6	3,703	0.036
Cora	Citation network	2,708	5,429	7	1,433	0.052
Pubmed	Citation network	19,717	44,338	3	500	0.003
NELL	Knowledge graph	65,755	266,144	210	5,414	0.001

(Kipf & Welling, Semi-Supervised Classification with Graph Convolutional Networks, ICLR 2017)

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Classification results (accuracy)

no input features

Method	Citeseer	Cora	Pubmed	NELL
ManiReg [3]	60.1	59.5	70.7	21.8
SemiEmb [24]	59.6	59.0	71.1	26.7
LP [27]	45.3	68.0	63.0	26.5
DeepWalk [18]	43.2	67.2	65.3	58.1
Planetoid* [25]	64.7 (26s)	75.7 (13s)	77.2 (25s)	61.9 (185s)
GCN (this paper)	**70.3** (7s)	**81.5** (4s)	**79.0** (38s)	**66.0** (48s)
GCN (rand. splits)	67.9 ± 0.5	80.1 ± 0.5	78.9 ± 0.7	58.4 ± 1.7

(Kipf & Welling, Semi-Supervised Classification with Graph Convolutional Networks, ICLR 2017)

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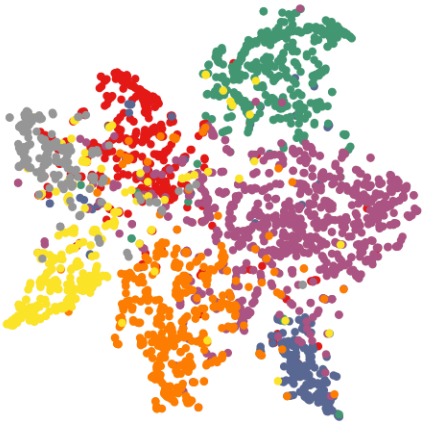


Learned representations
(t-SNE embedding of hidden layer activations)

Datas				l rate
Citese				0.036
Cora				0.052
Pubme				0.003
NELL				0.001

				LL
				8
				7
[27]				5
DeepWalk [18]	43.2	67.2	65.3	58.1
Planetoid* [25]	64.7 (26s)	75.7 (13s)	77.2 (25s)	61.9 (185s)
GCN (this paper)	**70.3** (7s)	**81.5** (4s)	**79.0** (38s)	**66.0** (48s)
GCN (rand. splits)	67.9 ± 0.5	80.1 ± 0.5	78.9 ± 0.7	58.4 ± 1.7

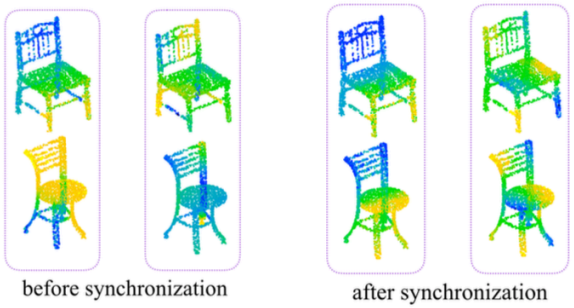
no input features

(Kipf & Welling, Semi-Supervised Classification with Graph Convolutional Networks, ICLR 2017)

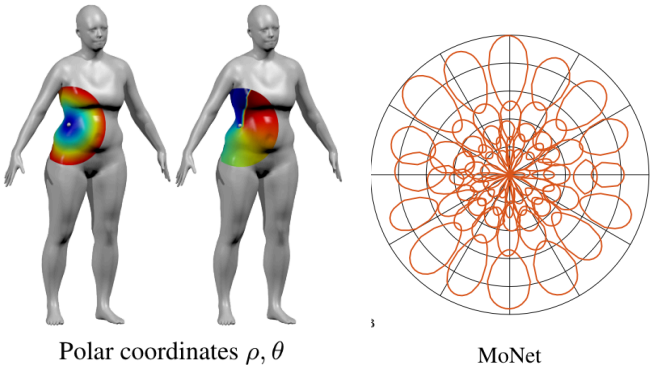
Other recent work

Global filters (hard to generalize) — Local filters (limited field of view)

Spectral domain ⟷ **Spatial domain**



SyncSpecCNN
(Spectral Transformer Nets)
[Yi et al., 2016]



Mixture model CNN
(learned basis functions)
[Monti et al., 2016]

$$g_\theta(\Lambda) = \sum_{k=0}^{K-1} \theta_k T_k(\tilde{\Lambda})$$

Chebyshev CNN (approximate spectral filters in spatial domain) [Defferrard et al., 2016]

Conclusions and open questions

Results from past 1-2 years have shown:

- Deep learning paradigm can be extended to graphs
- State-of-the-art results in a number of domains
- Use end-to-end training instead of multi-stage approaches
  (graph kernels, DeepWalk, node2vec etc.)

Open problems:

- Learn basis functions from scratch - First step: [Monti et al., 2016]
- Robustness of filters to change of graph structure
- Learn representations of graphs - First step: [Duvenaud et al., 2015]
- Theoretical understanding of what is learned
- Common benchmark datasets
- …

Further reading

Blog post Graph Convolutional Networks:
http://tkipf.github.io/graph-convolutional-networks

Code on Github:
http://github.com/tkipf/gcn

Kipf & Welling, Semi-Supervised Classification with Graph Convolutional Networks, ICLR 2017:
https://arxiv.org/abs/1609.02907

Kipf & Welling, Variational Graph Auto-Encoders, NIPS BDL Workshop, 2016:
https://arxiv.org/abs/1611.07308

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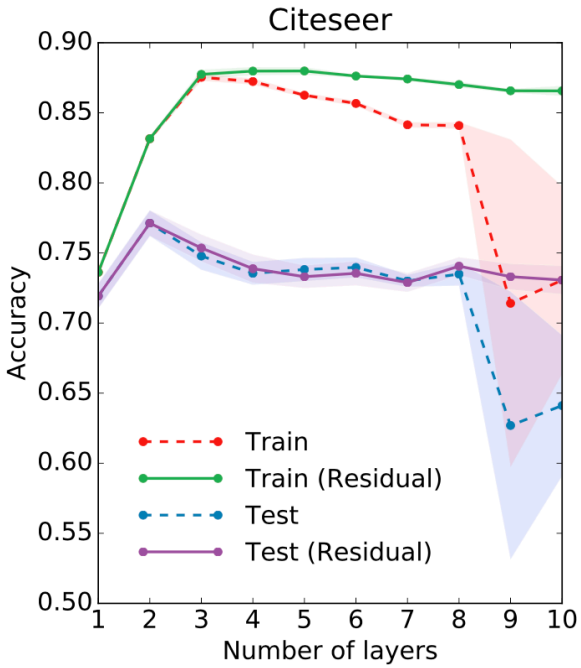
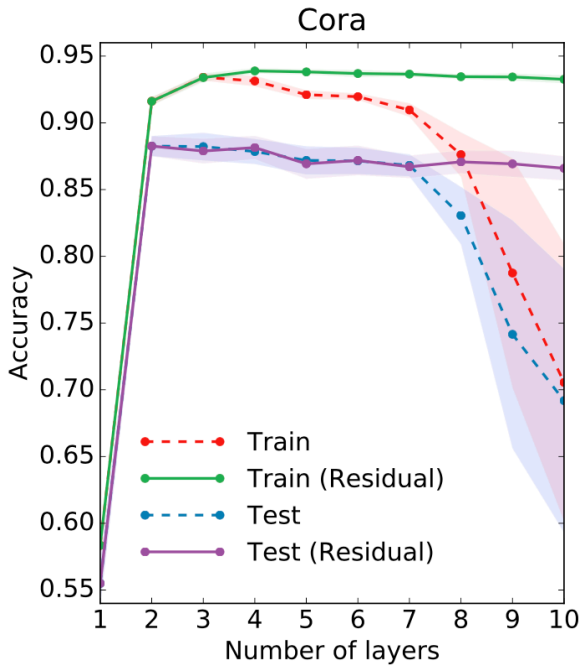
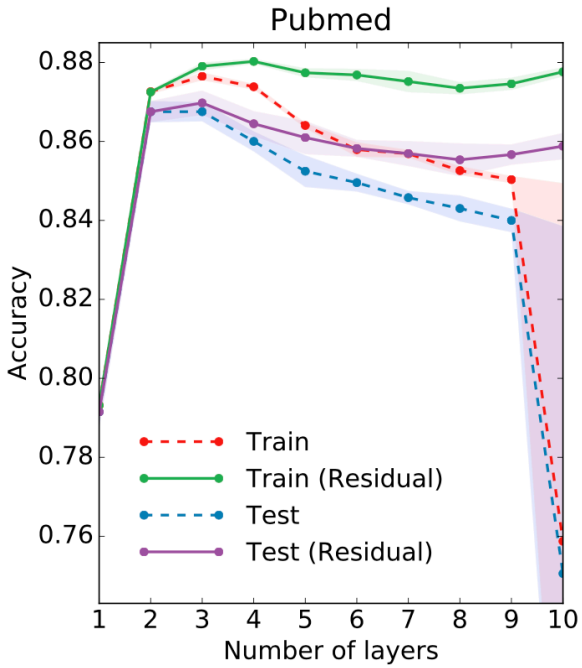
How deep is deep enough?







Residual connection

$$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)}\right) + H^{(l)}$$