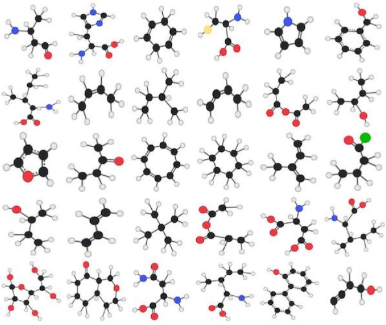
Neural Networks on Graphs

Machine Learning
Federico Magnolfi & Niccolò Biondi
Prof. Paolo Frasconi

20 April 2020

Overview

Graphs



Many **application domains** Many **tasks**

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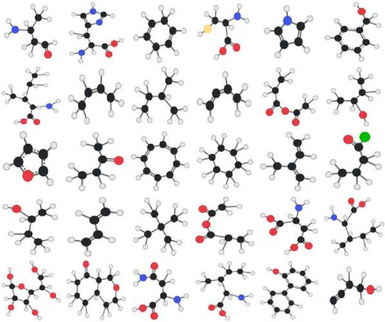

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Many **tasks**

- graph classification

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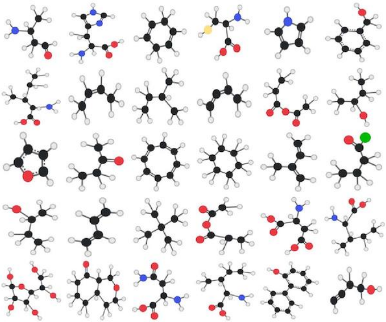


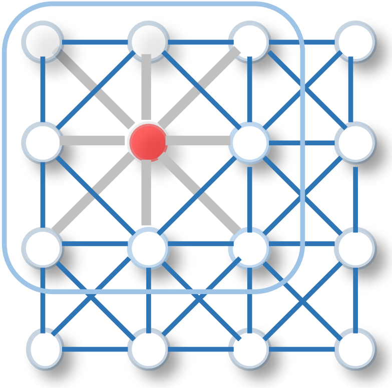
Many **application domains**

- chemistry
- social networks

Many **tasks**

- graph classification
- node classification

Graphs: difficulties



Images

- **regular** structure
- **ordered** neighbors

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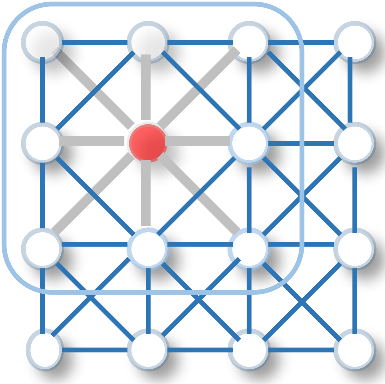

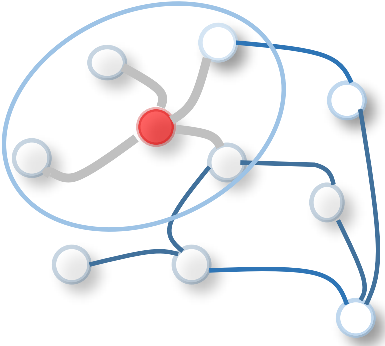

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Graphs

- **irregular** structure
- **unordered** neighbors

Some definitions

Graph: $\mathcal{G} = (A, X)$

- Adjacency matrix: A
- Feature matrix: X

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Remark

A sparse $\Rightarrow$ L sparse

Objective of this project

Objective

Reproduce some **experimental results** of 4 papers
on three different datasets

1. Planetoid (Yang et al., 2016)
2. ChebNet (Defferrard et al., 2016)
3. GCN (Kipf & Welling et al., 2017)
4. GAT (Veličković et al., 2018)

All these algorithms:

- use **Neural Networks**
- to **predict node class**
- in a **semi-supervised** setting

Datasets: citation networks

	Cora	**Citeseer**	**Pubmed**
# **Nodes**	2708	3327	19717
# **Edges**	5429	4732	44338
# **Features/Node**	1433	3703	500
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# Training Nodes	140	120	60
# Validation Nodes	500	500	500
# Test Nodes	1000	1000	1000

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Chebychev Networks

(Defferrard et al., 2016)

Spectral Convolutional GNN

Assume the graph is undirected

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Problems

1. N parameters per filter
2. filters not localized in space

Chebychev Networks (ChebNets)

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Spectral ConvGNN that obtains g_θ from **Chebychev polynomials** of $\widetilde{\Lambda}$

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Chebychev layer

$\theta \in \mathbb{R}^K$ $T_k(\widetilde{L}) \in \mathbb{R}^{N \times N}$ $x \in \mathbb{R}^N$

Single-filter, single-feature

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$$G_\Theta * X = \sum_{k=0}^{K-1} T_k(\widetilde{L}) X \Theta_k$$

- T_k: cheb polynomial of order k
- X: input
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Considerations

- $T_k(\widetilde{L})X$: is a sparse-dense matmul
- $[T_k(\widetilde{L})X]\Theta_k$: is a dense matmul
- efficiently computed on parallel architectures

Graph Convolutional Networks

(Kipf & Welling, 2017)

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Definition

$$M \triangleq \widetilde{D}^{-\frac{1}{2}} \widetilde{A} \widetilde{D}^{-\frac{1}{2}}$$

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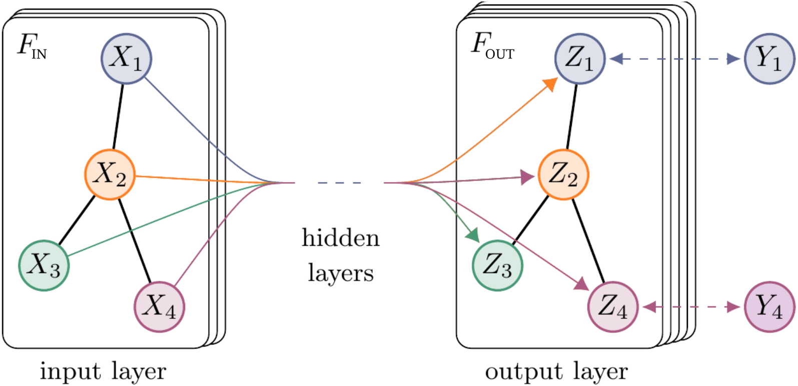

Experimental Setup

Preprocessing

- row-normalize X

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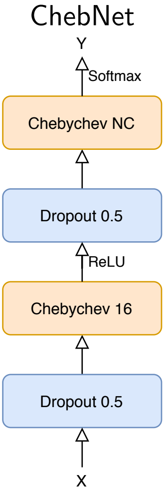

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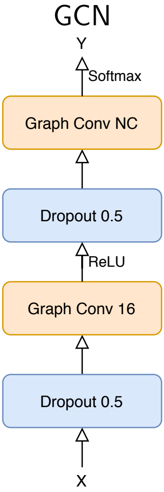

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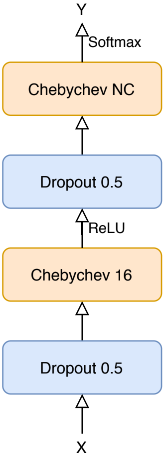

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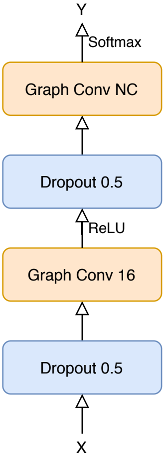

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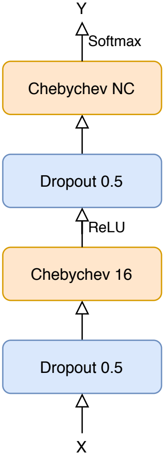

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Evaluation

- metric: accuracy on test nodes

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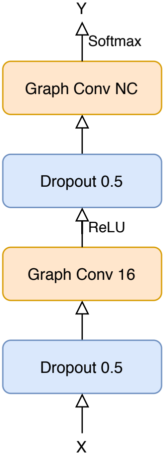

Results for ChebNet and GCN

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ChebNet*	$82.0 \pm 0.6\%$	$70.5 \pm 0.7\%$	$75.2 \pm 1.8\%$

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(Yang et al., 2016)

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Semi-supervised framework loss

$$\mathcal{L} = \mathcal{L}_s + \lambda \mathcal{L}_u$$

$$\mathcal{L}_s = -\sum_{i=0}^{N} \sum_{j=0}^{K} y_{ij} log(\hat{y}_{ij})$$

$\mathcal{L}_u \Rightarrow$ Embedding vs Laplacian regularization

Planetoid Contributions

- Embeddings exploited on several points of view:
  - are incorporated into graph **semi-supervised task**
  - to learn the **distributional context** of instances
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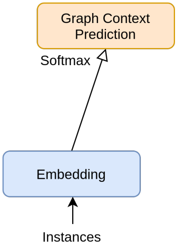
Proposed Frameworks

- Planetoid-T $\Rightarrow$ Transductive
- Planetoid-I $\Rightarrow$ Inductive

Embeddings

- Softmax layer on embeddings w.r.t. all nodes
- *Similar* instances close in embedding space
  - nearby nodes in the graph
  - nodes with same labels



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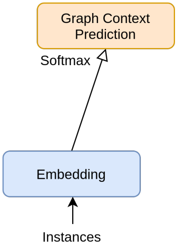


Embedding loss

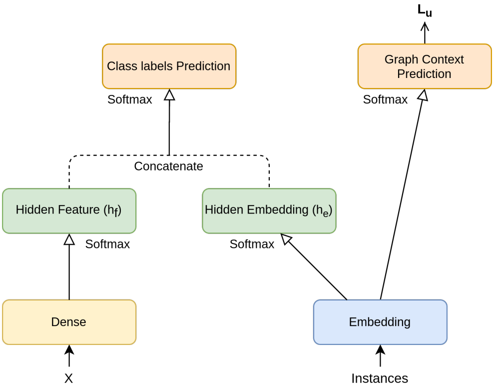
Embedding learning methods minimize the **log loss** of predicting context from the embedding of an instance (Skipgram model)

$$\mathcal{L}_u = -\sum_{(i,c)} \log p(c|i) = -\sum_{(i,c)} \log \left(\frac{\exp(\mathbf{w}_c^T \mathbf{e}_i)}{\sum_{c' \in \mathcal{C}} \exp(\mathbf{w}_{c'}^T \mathbf{e}_i)} \right)$$

Planetoid-T

Two phases

1. **pre-train**
2. training

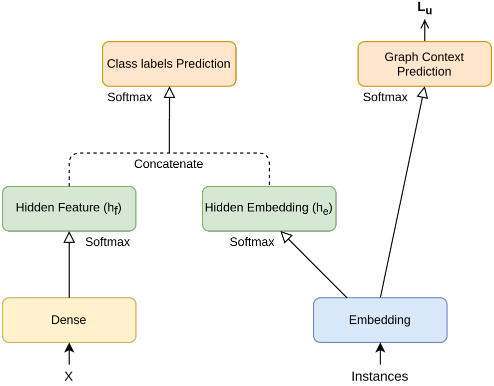


- Pretrained Embeddings leveraged during labels classification

Planetoid-T

Two phases

1. pre-train
2. **training**



- Pretrained Embeddings leveraged during labels classification

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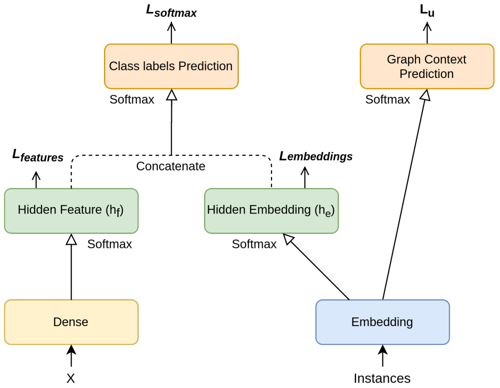

- Pretrained Embeddings leveraged during labels classification
- Total model loss: $\mathcal{L} = \mathcal{L}_s = \mathcal{L}_{softmax} + \mathcal{L}_{features} + \mathcal{L}_{embeddings}$

Planetoid-I

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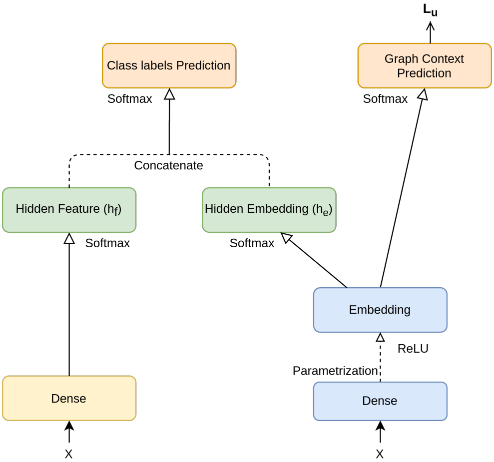

- Embeddings as a parameterized function of feature vectors

Planetoid-I

Two phases

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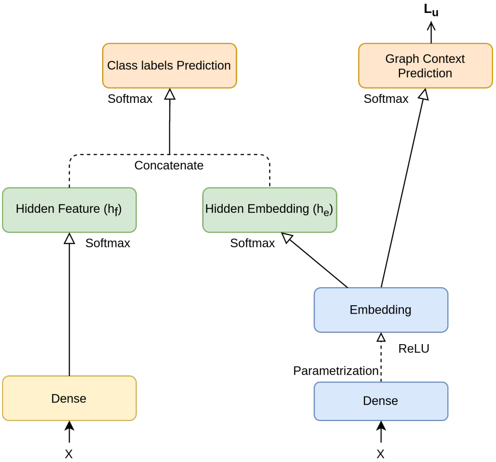

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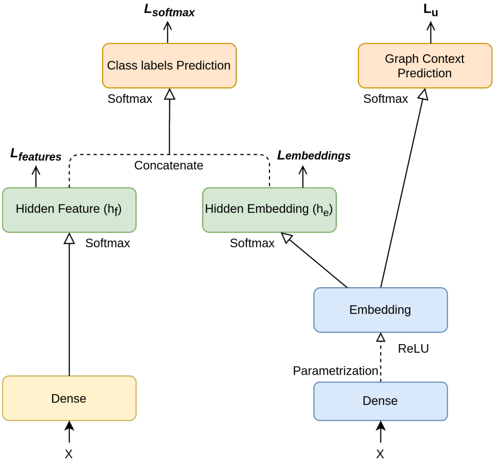

- Embeddings as a parameterized function of feature vectors
- Total model loss: $\mathcal{L} = \mathcal{L}_s + \lambda\mathcal{L}_u$

Experimental Results

Method	Cora	Citeseer	Pubmed
Planetoid	75.7%	64.7%	77.2%
Planetoid*	$73.1 \pm 0.9\%$	$62.3 \pm 1.1\%$	$73.5 \pm 0.7\%$

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- The authors validate the model on test set
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Planetoid***(max)**	77.2 %	66.2 %	75.9 %

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Graph Attention Networks

(Veličković et al., 2018)

GAT Contributions

Anisotropy

- Attention to give **different importance** to **neighbors**
- Attention mechanism is **shared** to all nodes
  - no dependency on graph structure
  - graphs can be directed

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Considerations

- No spectral convolution
- Sparse and parallel computations (high efficiency)

Attention Layer

Layer Configuration

- Input: $\mathbf{h} = \{\vec{h}_1, \vec{h}_2, \ldots, \vec{h}_N\}, \vec{h}_i \in \mathbb{R}^F$
- Output: $\mathbf{h}' = \{\vec{h}'_1, \vec{h}'_2, \ldots, \vec{h}'_N\}, \vec{h}'_i \in \mathbb{R}^{F'}$

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1. Normalized Attention Coefficients
2. Attention Layer Activation

Attention Layer: Coefficients

For each node i and its neighborhood ($\forall j \in \mathcal{N}_i$):

Attention Coefficient

$$e_{ij} = a(\mathbf{W}\vec{h}_i, \mathbf{W}\vec{h}_j)$$

- $\mathbf{W} \in \mathbb{R}^{F' x F}$ linear transformation
- Attentional mechanism parametrized by $\mathbf{a} \in \mathbb{R}^{2F'}$

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Normalized Attention Coefficient

$$\alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k \in \mathcal{N}_i} \exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_k]\right)\right)}$$

Attention Layer: Activation

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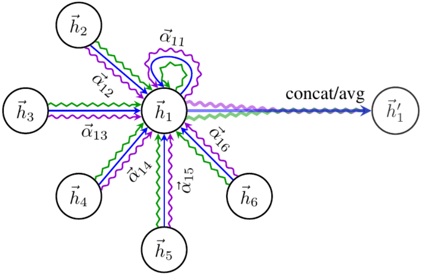

GAT model

Preprocessing

- row-normalize X

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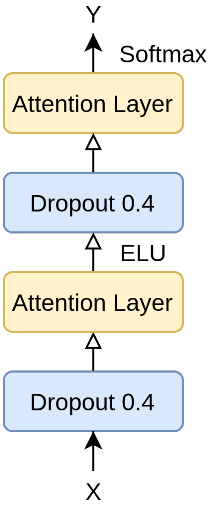
Model



GAT model

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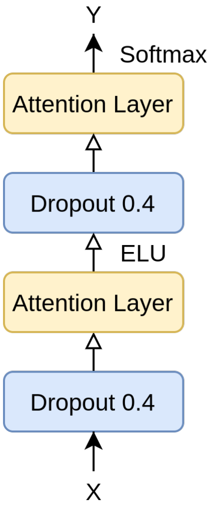
- loss: *categorical cross-entropy*
- regularization: L2 on model weights
- hyperparameters: different heads numbers



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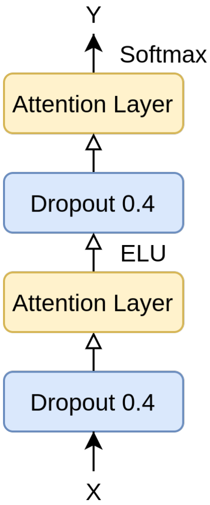
Evaluation

- metric: classification accuracy on test set



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Method	Cora	Citeseer	Pubmed
GAT	$83.0 \pm 0.7\%$	$72.5 \pm 0.7\%$	$79.0 \pm 0.3\%$
GAT*	$83.1 \pm 0.4\%$	$71.7 \pm 0.7\%$	$77.7 \pm 0.4\%$

*: (our) 100 runs, Yang data split, *optimization std*

Conclusions

Experimental Results

Method	Cora	Citeseer	Pubmed
Planetoid	75.7%	64.7%	77.2%
Planetoid*	$73.1 \pm 0.9\%$	$62.3 \pm 1.1\%$	$73.5 \pm 0.7\%$
Planetoid**	$72.3 \pm 2.0\%$	$59.4 \pm 2.0\%$	$69.7 \pm 2.8\%$

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Experimental Results

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Planetoid**	72.3 ± 2.0%	59.4 ± 2.0%	69.7 ± 2.8%
ChebNet	81.2%	69.8%	74.4%
ChebNet*	82.0 ± 0.6%	70.5 ± 0.7%	75.2 ± 1.8%
ChebNet**	78.9 ± 1.8%	68.2 ± 1.9%	73.4 ± 2.4%

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ChebNet**	78.9 ± 1.8%	68.2 ± 1.9%	73.4 ± 2.4%
GCN	81.5%	70.3%	79.0%
GCN*	80.6 ± 0.6%	68.7 ± 0.9%	78.3 ± 0.5%
GCN**	79.2 ± 1.7%	68.0 ± 1.8%	76.2 ± 2.5%
GAT	83.0 ± 0.7%	72.5 ± 0.7%	79.0 ± 0.3%
GAT*	83.1 ± 0.4%	71.7 ± 0.7%	77.7 ± 0.4%
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Next

- Better benchmark framework for GNNs
- More realistic data split

Thanks for the attention

References I

Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst, *Convolutional neural networks on graphs with fast localized spectral filtering*, 2016.

Vijay Prakash Dwivedi, Chaitanya K. Joshi, Thomas Laurent, Yoshua Bengio, and Xavier Bresson, *Benchmarking graph neural networks*, 2020.

P. Frasconi, M. Gori, and A. Sperduti, *A general framework for adaptive processing of data structures*, IEEE Transactions on Neural Networks **9** (1998), no. 5, 768–786.

C. Giles, Kurt Bollacker, and Steve Lawrence, *Citeseer: An automatic citation indexing system*, Proceedings of 3rd ACM Conference on Digital Libraries (2000).

M. Gori, G. Monfardini, and F. Scarselli, *A new model for learning in graph domains*, Proceedings. 2005 IEEE International Joint Conference on Neural Networks, 2005., vol. 2, 2005, pp. 729–734 vol. 2.

- Thomas N. Kipf and Max Welling, *Semi-supervised classification with graph convolutional networks*, 2016.
- A.K. McCallum, *Automating the construction of internet portals with machine learning*, Information Retrieval **3** (2000), 127–163.
- Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio, *Graph attention networks*, 2017.
- Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and Philip S. Yu, *A comprehensive survey on graph neural networks*, IEEE Transactions on Neural Networks and Learning Systems (2020), 1–21.
- Zhilin Yang, William W. Cohen, and Ruslan Salakhutdinov, *Revisiting semi-supervised learning with graph embeddings*, 2016.