

Deep Learning9. Graph Convolutions and Graph Attention

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Syllabus



Tue. 21.4.	(1)	1. Supervised Learning (Review 1)
Tue. 28.4.	(2)	2. Neural Networks (Review 2)
Tue. 5.5.	(3)	3. Regularization for Deep Learning
Tue. 12.5.	(4)	4. Optimization for Training Deep Models
Tue. 19.5.	(5)	5. Convolutional Neural Networks
Tue. 26.5.	(6)	6. Recurrent Neural Networks
Tue. 2.6.	—	— Pentecoste Break —
Tue. 9.6.	(7)	7. Autoencoders
Tue. 16.6.	(8)	ctd.
Tue. 23.6.	(9)	8. Attention Layers
Tue. 30.6.	(10)	9. Graph Convolutions and Graph Attention
Tue. 7.7.	(11)	10. Generative Adversarial Networks
Tue. 14.7.	(12)	Q & A

Outline



- 1. Supervised Learning for Graphs
- 2. Recurrent Graph Networks
- 3. Graph Convolutions
- 4. Graph Attention
- 5. Set-valued Inputs (DeepSet)

Outline



1. Supervised Learning for Graphs

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Graphs



any set V (called **vertices**) together with $E \subseteq V \times V$ (called **edges**)

- ► undirected graph G := (V, E): any set V (called vertices) together with E ⊆ subsets(V, card = 2) (called edges)
 - equivalent to a directed graph with symmetric edges,
 i.e., with E [!] = {(w, v) | (v, w) ∈ E}.
- vertex attributes $x^{vrt} \in \mathbb{R}^{V \times M^{vrt}}$
- edge attributes $x^{edge} \in \mathbb{R}^{E \times M^{edge}}$



Some Notation for Graphs



$$\mathcal{N}(v) := \{w \in V \mid \{v, w\} \in E\}$$

• fanin and fanout neighborhood of a vertex $v \in V$ in a directed graph:

$$\mathcal{N}_{in}(v) := \{ w \in V \mid (w, v) \in E \}$$
$$\mathcal{N}_{out}(v) := \{ w \in V \mid (v, w) \in E \}$$

► Denote the set of graphs with M^{vrt} vertex features and M^{edge} edge features (both possibly none) by

$$graphs(M^{vrt}, M^{edge})$$



Graph Classification



Given a set D^{train} ⊂ graphs(M^{vrt}, M^{edge}) × ℝ^O of pairs of graphs x_n = (V_n, E_n) and targets y_n ∈ ℝ^O and a pairwise loss ℓ : ℝ^O × ℝ^O → ℝ on targets find a prediction model

 $\hat{y} : \mathsf{graphs}(M^{\mathsf{vrt}}, M^{\mathsf{edge}}) \to \mathbb{R}^O$

with minimal loss for test data $\mathcal{D}^{\text{test}} \subset \text{graphs}(M^{\text{vrt}}, M^{\text{edge}}) \times \mathbb{R}^{O}$ (from the same distribution):

$$\ell(\hat{y}; \mathcal{D}^{\mathsf{test}}) := \frac{1}{|\mathcal{D}^{\mathsf{test}}|} \sum_{(V, E, y) \in \mathcal{D}^{\mathsf{test}}} \ell(y, \hat{y}(V, E))$$

Vertex Classification (aka Node Classification)

 vertex features x^{vrt} are partitioned into two groups, vertex predictors and vertex targets:

 $x^{\mathsf{vrt}} = \mathsf{concat}_2(ilde{x}, y), \quad ilde{x} \in \mathbb{R}^{V imes M}, y \in \mathbb{R}^{V imes O}$

• given the graph (V, E),

all vertex predictors \tilde{x} ,

a random subset of vertex targets $y|_{V^{\text{train}}}$, $V^{\text{train}} \subset V$, and a pairwise loss $\ell : \mathbb{R}^O \times \mathbb{R}^O \to \mathbb{R}$ on targets,

find a prediction $\hat{y} \in \mathbb{R}^{V^{\text{test}} \times O}$ of the remaining vertex targets $V^{\text{test}} := V \setminus V^{\text{train}}$ s.t. their loss w.r.t. the true targets is minimal:

$$\ell(\hat{y}; y) := rac{1}{|V^{ ext{test}}|} \sum_{v \in V^{ ext{test}}} \ell(y_v, \hat{y}_v)$$

- ► called a transductive problem, because
 - ► no model function ŷ is sought, that predicts targets individually for every instance/node,
 - but just the target values for a fixed set of predictors predicted collectively



A New Problem?



Q: Can we solve vertex classification like any other classification problem?

A New Problem?



- Q: Can we solve vertex classification like any other classification problem?
- ► Is there also an edge classification problem?

Line Graphs



• line graph of a graph G := (V, E):

line
$$(V, E) := (E, \{\{e, f\} \subset E \mid |e \cap f| = 1\})$$

- each original edge becomes a vertex.
- two edges are connected by an edge, if originally they are connected by a vertex.



[source: wikipedia/line_graph]

Line Graphs / Features



- $G := (V, E), \tilde{G} := \text{line}(V, E)$
- ► edges become vertices ~>> edge features become vertex features:

$$ilde{x}_e^{\mathsf{vrt}} := x_e^{\mathsf{edge}}, \quad e \in E$$

► vertices become edges ~~ vertex features become edge features:

$$\widetilde{x}_{e,f}^{\mathsf{edge}} := x_{e\cap f}^{\mathsf{vrt}} \quad e,f \in E$$

beware, a vertex can become many edges, thus all the edges represented by the same original vertex have the same features.

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Edge Classification?

- ► Is there also an edge classification problem?
- ► practically: sure.
- ► methododically: no, it is not a new problem.
 - edge classification is the same as vertex classification for the line graph.

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- 2. Recurrent Graph Networks
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Graph Neural Networks



$$z_{v} \stackrel{!}{=} \sum_{w \in \mathcal{N}(v)} h(z_{v}, z_{w}, x_{v}^{\mathsf{vrt}}, x_{w}^{\mathsf{vrt}}, x_{v,w}^{\mathsf{edge}})$$
$$y_{v} := g(z_{v}, x_{v}^{\mathsf{vrt}})$$

- ► g, h fully connected neural networks
- ► Q: How can we compute the latent features?

► Scarselli et al. [2008]



(1)

Graph Neural Networks



(1)

• recurrent latent vertex features $z_v \in \mathbb{R}^K$:

$$z_{v} \stackrel{!}{=} \sum_{w \in \mathcal{N}(v)} h(z_{v}, z_{w}, x_{v}^{vrt}, x_{w}^{vrt}, x_{v,w}^{edge})$$
$$y_{v} := g(z_{v}, x_{v}^{vrt})$$

- ► g, h fully connected neural networks
- z_v have to be computed as fixpoints of eq. 1
- ▶ thus *h* needs to be chosen with care: to be contractive.
- ► Scarselli et al. [2008]

Gated Graph Sequence Neural Networks

- ▶ two types of latent vertex features $z_v, h_v \in \mathbb{R}^K$
 - ► stacking several layers: $z_v^t, h_v^t, t = 1, ..., T$ $h_v^0 := x_v^{\text{vrt}}$, padded with zeros.
- latent vertex features $z^t \in \mathbb{R}^{V \times K}$:

 $z_{v}^{t+1} := (h^{t})^{T} (x_{v,...}^{\text{edge}} w^{\text{out}} + x_{..v,..}^{\text{edge}} w^{\text{in}}), \quad w^{\text{out}}, w^{\text{in}} \in \mathbb{R}^{M^{\text{edge}}}$ $\blacktriangleright \text{ representing the edge features as array } x^{\text{edge}} \in \mathbb{R}^{V \times V \times M^{\text{edge}}}$ (being zero for non-edges)

- ▶ based on all previous latent vertex features $h^t \in \mathbb{R}^{V \times K}$
- ► latent vertex features $h^t \in \mathbb{R}^{V \times K}$, computed via a GRU RNN:

$$h_v^t := \mathsf{GRU}(z_v^t, h_v^{t-1})$$

- using z^t instead of the sequence inputs x^t as done usually.
- being applied to each vertex in isolation!
- ▶ Li et al. [2015]



Gated Graph Sequence Neural Networks



$$z_v^{t+1} := (h^t)^T (x_{v,.,.}^{\mathsf{edge}} w^{\mathsf{out}} + x_{.,v,.}^{\mathsf{edge}} w^{\mathsf{in}}), \quad w^{\mathsf{out}}, w^{\mathsf{in}} \in \mathbb{R}^{M^{\mathsf{edge}}}$$

► make it simple: no edge features, i.e., M^{edge} := 1 and x^{edge}_{...,1} = A is just the adjacency matrix.

$$z_v^{t+1} = w^{\mathsf{out}} \sum_{u \in \mathcal{N}_{\mathsf{out}}(v)} h_u^t + w^{\mathsf{in}} \sum_{u \in \mathcal{N}_{\mathsf{in}}(v)} h_u^t$$

 i.e, this is DeepSet for the fanin and fanout neighborhoods. (before DeepSet was invented, that is.)



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Papers on Graph Convolutions (source: Zhang et al. [2020])



Method	Туре	Convolution	Readout	T.C.	M.G.	Other Characteristics
Bruna et al. [40]	Spectral	Interpolation kernel	Hierarchical clustering + FC	$O(N^{3})$	No	-
Henaff et al. [41]	Spectral	Interpolation kernel	Hierarchical clustering + FC	$O(N^3)$	No	Constructing the graph
ChebNet [42]	Spectral/Spatial	Polynomial	Hierarchical clustering	O(M)	Yes	
Kipf&Welling [43]	Spectral/Spatial	First-order	-	O(M)	-	-
CayletNet [44]	Spectral	Polynomial	Hierarchical clustering + FC	O(M)	No	-
GWNN [45]	Spectral	Wavelet transform	-	O(M)	No	-
Neural FPs [46]	Spatial	First-order	Sum	O(M)	Yes	-
PATCHY-SAN [47]	Spatial	Polynomial + an order	An order + pooling	$O(M \log N)$	Yes	A neighbor order
LGCN [48]	Spatial	First-order + an order	-	O(M)	Yes	A neighbor order
SortPooling [49]	Spatial	First-order	An order + pooling	O(M)	Yes	A node order
DCNN [50]	Spatial	Polynomial diffusion	Mean	$O(N^2)$	Yes	Edge features
DGCN [51]	Spatial	First-order + diffusion	-	$O(N^2)$	-	-
MPNNs [52]	Spatial	First-order	Set2set	O(M)	Yes	A general framework
GraphSAGE [53]	Spatial	First-order + sampling	-	$O(Ns^L)$	Yes	A general framework
MoNet [54]	Spatial	First-order	Hierarchical clustering	O(M)	Yes	A general framework
GNs [9]	Spatial	First-order	A graph representation	O(M)	Yes	A general framework
Kearnes et al. [55]	Spatial	Weave module	Fuzzy histogram	O(M)	Yes	Edge features
DiffPool [56]	Spatial	Various	Hierarchical clustering	$O(N^2)$	Yes	Differentiable pooling
GAT [57]	Spatial	First-order	-	O(M)	Yes	Attention
GaAN [58]	Spatial	First-order	-	$O(Ns^L)$	Yes	Attention
HAN [59]	Spatial	Meta-path neighbors	-	$O(M_{\phi})$	Yes	Attention
CLN [60]	Spatial	First-order	-	O(M)	-	-
PPNP [61]	Spatial	First-order	-	O(M)	-	Teleportation connections
JK-Nets [62]	Spatial	Various	-	O(M)	Yes	Jumping connections
ECC [63]	Spatial	First-order	Hierarchical clustering	O(M)	Yes	Edge features
R-GCNs [64]	Spatial	First-order	-	O(M)	-	Edge features
LGNN [65]	Spatial	First-order + LINE graph	-	O(M)	-	Edge features
PinSage [66]	Spatial	Random walk	-	$O(Ns^L)$	-	Neighborhood sampling
StochasticGCN [67]	Spatial	First-order + sampling	-	$O(Ns^L)$	-	Neighborhood sampling
FastGCN [68]	Spatial	First-order + sampling	-	O(NsL)	Yes	Layer-wise sampling
Adapt [69]	Spatial	First-order + sampling	-	O(NsL)	Yes	Layer-wise sampling
Li et al. [70]	Spatial	First-order	-	O(M)	-	Theoretical analysis
SGC [71]	Spatial	Polynomial	-	O(M)	Yes	Theoretical analysis
GFNN [72]	Spatial	Polynomial	-	O(M)	Yes	Theoretical analysis
GIN [73]	Spatial	First-order	Sum + MLP	O(M)	Yes	Theoretical analysis
DGI [74]	Spatial	First-order	-	O(M)	Yes	Unsupervised training

Deep Locally Connected Networks



- ▶ the vertices of the graph are partitioned into *S* clusters C_1, \ldots, C_S
- vertex cluster latent features $z_s \in \mathbb{R}^K$:

$$z_{s,k}^{\ell+1} := \sum_{v \in C_s} h(\sum_{j=1}^{K} W_{k,j}^{\ell+1} z_{v,j}^{\ell}) \quad s = 1, \dots, S, \ j = 1, \dots, K, \ W^{\ell+1} \in \mathbb{R}^{K \times K}$$

- $h: \mathbb{R}^K \to \mathbb{R}^K$ is a suitable function (unspecified)
- What actually does $h(\sum_{j=1}^{K} W_{k,j}^{\ell} z_{v,j}^{\ell})$?

▶ Bruna et al. [2013]

Deep Locally Connected Networks



- ▶ the vertices of the graph are partitioned into *S* clusters C_1, \ldots, C_S
- vertex cluster latent features $z_s \in \mathbb{R}^K$:

$$z_{s,k}^{\ell+1} := \sum_{v \in C_s} h(\sum_{j=1}^{K} W_{k,j}^{\ell+1} z_{v,j}^{\ell}) \quad s = 1, \dots, S, \ j = 1, \dots, K, \ W^{\ell+1} \in \mathbb{R}^{K \times K}$$

- $h: \mathbb{R}^{K} \to \mathbb{R}^{K}$ is a suitable function (unspecified)
- instead of summing over C_s , the paper talks just about "pooling".
- vertex clusters are assembled to a new graph with weighted edges, by summing and normalizing the weights between vertices of each two clusters.
- ► Bruna et al. [2013]



Spectral Networks

• vertex latent features $z \in \mathbb{R}^{V \times K}$:

$$z_{.,k}^{\ell+1} := a(\sum_{j=1}^{K} Q \operatorname{diag}(W_{k,j}^{\ell+1}) Q^{T} z_{.,j}^{\ell}), \quad W_{k,j}^{\ell-1} \in \mathbb{R}^{V}$$

- $x^{\text{edge}} \in \mathbb{R}^{V \times V}$ symmetric, $x^{\text{edge}} \ge 0$ edge weights
- ► Lap := diag(x^{edge}1) x^{edge} Weighted Graph Laplacian
- ► $Q \in \mathbb{R}^{V \times V}$ the eigenvector matrix of the Laplacian: Lap $\stackrel{!}{=} Q \operatorname{diag}(\lambda)Q^{T}, \quad \lambda \in \mathbb{R}^{V}$
- ▶ Bruna et al. [2013]

Spectral Networks / Filter Parametrization



- ▶ how are the filters $W_{k,j}^{\ell-1} \in \mathbb{R}^V$ parametrized (k, j = 1, ..., K) ?
 - ▶ let's use just $W \in \mathbb{R}^V$ to denote $W_{k,j}^{\ell-1}$ on this slide
- non-parametric filter (not used):

$$W = \theta \in \mathbb{R}^V$$

▶ interpolation from fixed size filter $\theta \in \mathbb{R}^L$, $L \ll V$ with a cubic spline:

$$W(heta) = \mathsf{qsk}(V) heta, \hspace{1em} \mathsf{qsk}(V) \in \mathbb{R}^{V imes L}$$
 cubic spline kernel

▶ polynom in the eigenvalues $\lambda \in \mathbb{R}^V$ of the Laplacian:

$$W(\lambda; heta) = \sum_{d=0}^{D-1} heta_d \lambda^d, \quad heta \in \mathbb{R}^D, D \in \mathbb{N} ext{ degree}$$

▶ Defferrard et al. [2016]

Note: Here λ^d denotes elementwise powers: $\lambda^d := (\lambda^d_v)_{v=1:V}$.

Deep Learning 3. Graph Convolutions

Experiments / Subsampled MNIST



[source: Bruna et al. [2013]]

Q: What you see?

Experiments / Subsampled MNIST



Table 1: Classification results on MNIST subsampled on 400 random locations, for different architectures. FCN stands for a fully connected layer with N outputs, LRFN denotes the locally connected construction from Section 2.3 with N outputs, MPN is a max-pooling layer with Noutputs, and SPN stands for the spectral layer from Section 3.2.

method	Parameters	Error
Nearest Neighbors	N/A	4.11
400-FC800-FC50-10	$3.6\cdot 10^5$	1.8
400-LRF1600-MP800-10	$7.2 \cdot 10^{4}$	1.8
400-LRF3200-MP800-LRF800-MP400-10	$1.6 \cdot 10^5$	1.3
400-SP1600-10 ($d_1 = 300, q = n$)	$3.2 \cdot 10^{3}$	2.6
400-SP1600-10 ($d_1 = 300, q = 32$)	$1.6\cdot 10^3$	2.3
400-SP4800-10 ($d_1 = 300, q = 20$)	$5 \cdot 10^3$	1.8

[source: Bruna et al. [2013]]

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Graph Attention Networks (GAT)



► restricted multi-head attention over the vertex neighborhood:

$$\operatorname{attnres}(X;\mathcal{N})_{v,u}:=\mathbb{I}(u\in\mathcal{N}(v)) ext{ attn}(X)_{v,u},\quad u,v\in V$$

using the vanilla attention mechanism:

$$\begin{aligned} \operatorname{attn}(X; w, v) &:= a(XW^T VX^T) \\ \operatorname{sha}(X; w, v, u) &:= \operatorname{attnres}(X; w, v) (XU^T) \\ \operatorname{mha}(X) &:= \operatorname{concat}_2((\operatorname{sha}(X_{1:V, \operatorname{slice}(h)}; w^h, v^h, u^h))_{h=1:H})Q^T, \\ Q \in \mathbb{R}^{K^{\operatorname{out}} \times HK} \end{aligned}$$

- with $X := x^{edge} \in \mathbb{R}^{V \times M^{edge}}$ the vertex features.
- ▶ Veličković et al. [2017]

Model Configuration

► 2 GAT layers

- 1. 8 heads à 8 features, exponential linear unit
- 2. 1 head à O features, softmax
- L2 regularization $\lambda = 0.0005$,

Dropout p = 0.6 for both layers' inputs and both layers' attention weights. (= random sub-neighborhood)

 has been optimized for first dataset (Cora), used unchanged for the other two.

▶ # parameters: Cora: 276k
Citeseer: 712k
Pubmed: 97k
Note: Exponential linear unit (ELU):
$$elu(z) := \begin{cases} x & \text{if } x \ge 0 \\ o(x^2 - 1) & olive \end{cases}$$
.



Experiments / Datasets



	Cora	Citeseer	Pubmed	PPI
Task	Transductive	Transductive	Transductive	Inductive
# Nodes	2708 (1 graph)	3327 (1 graph)	19717 (1 graph)	56944 (24 graphs)
# Edges	5429	4732	44338	818716
# Features/Node	1433	3703	500	50
# Classes	7	6	3	121 (multilabel)
# Training Nodes	140	120	60	44906 (20 graphs)
# Validation Nodes	500	500	500	6514 (2 graphs)
# Test Nodes	1000	1000	1000	5524 (2 graphs)

[source: Veličković et al. [2017]]

Experiments / Results



Transductive					
Method	Cora	Citeseer	Pubmed		
MLP	55.1%	46.5%	71.4%		
ManiReg (Belkin et al., 2006)	59.5%	60.1%	70.7%		
SemiEmb (Weston et al., 2012)	59.0%	59.6%	71.7%		
LP (Zhu et al., 2003)	68.0%	45.3%	63.0%		
DeepWalk (Perozzi et al., 2014)	67.2%	43.2%	65.3%		
ICA (Lu & Getoor, 2003)	75.1%	69.1%	73.9%		
Planetoid (Yang et al., 2016)	75.7%	64.7%	77.2%		
Chebyshev (Defferrard et al., 2016)	81.2%	69.8%	74.4%		
GCN (Kipf & Welling, 2017)	81.5%	70.3%	79.0%		
MoNet (Monti et al., 2016)	$81.7\pm0.5\%$	_	$78.8\pm0.3\%$		
GCN-64*	$81.4\pm0.5\%$	$70.9\pm0.5\%$	$\textbf{79.0} \pm 0.3\%$		
GAT (ours)	$\textbf{83.0}\pm0.7\%$	$\textbf{72.5} \pm 0.7\%$	$\textbf{79.0} \pm 0.3\%$		

[source: Veličković et al. [2017]]

Note: shown is microaveraged F1.

Experiments / Results



[source: paperswithcode.com]



Experiments / Results







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Set Function Representation Theorem

• let
$$\mathcal{X}, \mathcal{Y}$$
 be any sets, i.e., $\mathcal{X} := \mathbb{R}^M$, $\mathcal{Y} := \mathbb{R}^O$.

▶ any function on (finite/countable) sets of elements from X to Y,

 $f:\mathsf{sets}(\mathcal{X}) o \mathcal{Y}$

can be written as

$$f(X) = g(\sum_{x \in X} h(x))$$

for two suitable functions $h : \mathcal{X} \to \mathbb{R}^{K}, g : \mathbb{R}^{K} \to \mathcal{Y}$ and a suitable $K \in \mathbb{N}$.



⇐:



Set Function Representation Theorem / Proof

 $f(\pi(X)) = g(\sum_{x \in \pi(X)} h(x)) = g(\sum_{x \in X} h(x)) = f(X)$

 $\Rightarrow: \text{ here only for the case that } \mathcal{X} \text{ is countable,} \\ \text{ i.e., there exists a injective map } c: \mathcal{X} \to \mathbb{N}:$

$$\begin{split} h(x) &:= 4^{-c(x)}, \quad \mathcal{K} := 1 \\ &\rightsquigarrow \quad z(X) := \sum_{x \in X} h(x) \text{ is injective (4-ary code of } X) \\ &g(z) := f(z^{-1}(z)) \end{split}$$

and then:

$$g(\sum_{x \in \pi(X)} h(x)) = g(z(X)) = f(z^{-1}(z(X))) = f(X)$$

DeepSet



- ► invariant layer:
 - ► input: $x \in \mathbb{R}^{* \times M}$ ($\hat{=}$ { $x_1, x_2, ..., x_T$ }, $x_t \in \mathbb{R}^M$, number T of elements variable)
 - output: $z \in \mathbb{R}^{O}$

$$z(x) := g(\sum_{t=1}^{T} h(x_{t,.}))$$
$$h : \mathbb{R}^{M} \to \mathbb{R}^{K} \text{ element encoder}$$
$$g : \mathbb{R}^{K} \to \mathbb{R}^{O} \text{ decoder}$$

- ► aggregation of encoded elements by sum, mean, or max.
- ► Zaheer et al. [2017]

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Equivariant Layer

- ► equivariant layer:
 - ► input: $x \in \mathbb{R}^*$ ($\hat{=}$ { $x_1, x_2, ..., x_T$ }, $x_t \in \mathbb{R}$, number T of elements variable)
 - ▶ output: $z \in \mathbb{R}^*$ with same length

$$z(x) := a(cx + d(\max x)\mathbb{1}), \quad c, d \in \mathbb{R}$$

- ▶ formulated for $x \in \mathbb{R}^M$, i.e., for *M* scalar elements
- ► also $a(cx + d\mathbf{1}\mathbf{1}^T x)$ (sum) or $a(cx + d\frac{1}{|x|}\mathbf{1}\mathbf{1}^T x)$ (mean)

Summary



- (Transductive) vertex classification in a graph: given some labeled vertices, predict the targets/labels of the others.
- ► Early attempts to build neural networks for graphs used recurrent approaches
- Graph Convolutions aggregate vertex features
 - in the spectral domain: over vertex neighborhoods in the Eigenspace of the graph Laplacian.
 - ▶ in the spatial domain: over vertex neighborhoods in the graph directly.
- Graph Attention applies vanilla multi-head attention to the vertices, restricting it to their neighborhoods.
- Both, graph convolution networks and graph attention networks can be learned with vanilla backpropagation.
- Graph Attention Networks provide some of the best models currently for vertex classification.

Further Readings



- ► graph convolutions are not yet covered by the textbooks.
- ► see the referenced papers for details.
- ▶ surveys: Zhang et al. [2020]; Wu et al. [2020]; Kinderkhedia [2019]

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