Boulder

Graph Neural Networks

YouTube Playlist

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Translating Embeddings for Modeling Multi-relational Data

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Multi-relational Data

Directed graphs whose nodes correspond to entities and edges to relationships
$(h, \ell, t) \rightarrow$ there exists a relationship of name ℓ between the entities h and t
$h \rightarrow$ head, $\ell \rightarrow$ label, $t \rightarrow$ tail

– social network analysis:
  entities: members
  relationships: friendship/social relationship links
– recommender systems:
  entities: users and products
  relationships: buying, rating, reviewing and searching for a product
– knowledge bases (KBs):
  entities: abstract concepts or concrete entities of the world
  relationships: predicates that represent facts involving two entities

Freebase, Google Knowledge Graph, GeneOntology, WordNet
Link prediction: automatically add new facts without requiring extra knowledge

Translation-based Model

$S \rightarrow$ training set of triplets (h, ℓ, t)
$h, t \in E \rightarrow$ set of entities
$\ell \in L \rightarrow$ set of relationships
$v_e, v_\ell \in \mathbb{R}^k \rightarrow$ vector embeddings of the entities $e \in E$ and the relationships $\ell \in L$

Translation in the embedding space: Embedding v_t of the tail entity t should be close to the embedding v_h of the head entity h plus some vector v_ℓ that depends on the relationship ℓ.
We want $v_h + v_\ell \approx v_t$ when $(h, \ell, t) \in S$
$d \rightarrow$ dissimilarity measure (L_1 or L_2 norm)

$$\mathcal{L} = \sum_{(h,\ell,t)\in S} \sum_{(h',\ell,t')\in S'_{(h,\ell,t)}} [\gamma + d(v_h + v_\ell, v_t) - d(v_{h'} + v_\ell, v_{t'})]_+$$

$\gamma \rightarrow$ margin hyper-parameter

$$S'_{(h,\ell,t)} = \{(h', \ell, t) | h' \in E\} \cup \{(h, \ell, t') | t' \in E\}$$

$S'_{(h,\ell,t)} \rightarrow$ set of corrupted triplets

$\|v_e\|_2^2 = 1, \forall e \in E \rightarrow$ constraint

– easy to train
– reduced number of parameters
– scale up to very large datasets (1M entities, 25K relationships and more than 17M training examples)

```
For evaluation, use the following ranking procedure. For each test
triplet, the head is removed and replaced by each of the entities of
the dictionary in turn. Dissimilarities (or energies) of those
corrupted triplets are first computed by the models and then sorted by
ascending order; the rank of the correct entity is finally stored.
This whole procedure is repeated while removing the tail instead of
the head. Report the mean of those predicted ranks and the hits@10,
i.e. the proportion of correct entities ranked in the top 10.
```

Link prediction results. Test performance of the different methods.

Dataset	WN				FB15k				FB1M	
Metric	Mean Rank		Hits@10 (%)		Mean Rank		Hits@10 (%)		Mean Rank	Hits@10 (%)
Eval. setting	*Raw*	*Filt.*	*Raw*	*Filt.*	*Raw*	*Filt.*	*Raw*	*Filt.*	*Raw*	*Raw*
Unstructured [2]	315	304	35.3	38.2	1,074	979	4.5	6.3	15,139	2.9
RESCAL [11]	1,180	1,163	37.2	52.8	828	683	28.4	44.1	-	-
SE [3]	1,011	985	68.5	80.5	273	162	28.8	39.8	22,044	17.5
SME(linear) [2]	545	533	65.1	74.1	274	154	30.7	40.8	-	-
SME(bilinear) [2]	526	509	54.7	61.3	284	158	31.3	41.3	-	-
LFM [6]	469	456	71.4	81.6	283	164	26.0	33.1	-	-
TransE	**263**	**251**	**75.4**	**89.2**	**243**	**125**	**34.9**	**47.1**	**14,615**	**34.0**

WordNet (WN) & FreeBase (FB)

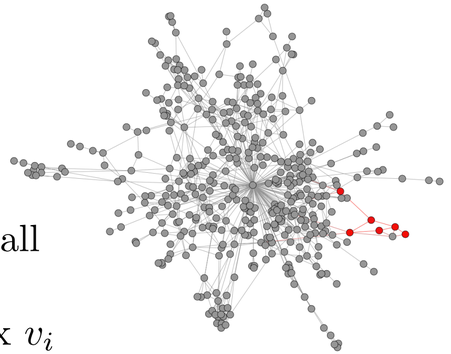
Bordes, Antoine, et al. "Translating embeddings for modeling multi-relational data." *Advances in neural information processing systems* 26 (2013).

DeepWalk: Online Learning of Social Representations

YouTube Video

Learning latent representations of vertices in a network
– BlogCatalog – Flickr – YouTube
– Network Classification – Anomaly Detection
– Content Recommendation – Missing Link Prediction

$G = (V, E) \rightarrow$ a social network
$V \rightarrow$ members of the network
$E \subset V \times V \rightarrow$ connections
$G_L = (V, E, X, Y) \rightarrow$ partially labeled social network



$X \in \mathbb{R}^{|V| \times S} \rightarrow$ attributes
$S \rightarrow$ size of the feature space
$Y \in \mathbb{R}^{|V| \times |\mathcal{Y}|}$
$\mathcal{Y} \rightarrow$ set of labels

Goal: Learn $X_E \in \mathbb{R}^{|V| \times d}$ with d small

Random Walks

$\mathcal{W}_{v_i} \rightarrow$ random walk rooted at vertex v_i
$\mathcal{W}_{v_i} \rightarrow$ stochastic process with random variables $\mathcal{W}_{v_i}^1, \mathcal{W}_{v_i}^2, \ldots$
$\mathcal{W}_{v_i}^{k+1} \rightarrow$ vertex chosen at random from neighbors of vertex $\mathcal{W}_{v_i}^k$

Language Modeling

$\Pr(v_i | v_1, \ldots, v_{i-1}) \rightarrow$ probability of observing vertex v_i given all the previous vertices visited so far in the random walk

$\Phi : v \in V \longmapsto \mathbb{R}^d$

Represent Φ by a matrix of free parameters $X_E \in \mathbb{R}^{|V| \times d}$

$\Pr(v_i | \Phi(v_1), \ldots, \Phi(v_{i-1})) \rightarrow$ unfeasible as the walk length grows

$$\underset{\Phi}{\text{minimize}} \quad -\log \Pr\left(\{v_{i-w}, \cdots, v_{i+w}\} \setminus v_i \mid \Phi(v_i)\right)$$

Algorithm 1 DeepWalk(G, w, d, γ, t)

Input: graph $G(V, E)$
window size w
embedding size d
walks per vertex γ $\rightarrow$ "epoch"
walk length t
Output: matrix of vertex representations $\Phi \in \mathbb{R}^{|V| \times d}$

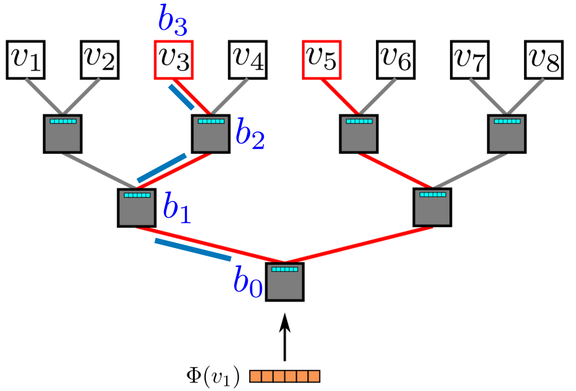
1: Initialization: Sample Φ from $\mathcal{U}^{|V| \times d}$
2: Build a binary Tree T from V
3: **for** $i = 0$ to γ **do**
4: $\quad \mathcal{O} = \text{Shuffle}(V)$
5: $\quad$ **for each** $v_i \in \mathcal{O}$ **do**
6: $\quad\quad \mathcal{W}_{v_i} = RandomWalk(G, v_i, t)$
7: $\quad\quad$ SkipGram(Φ, $\mathcal{W}_{v_i}$, w)
8: $\quad$ **end for**
9: **end for**

Algorithm 2 SkipGram(Φ, $\mathcal{W}_{v_i}$, w)

1: **for each** $v_j \in \mathcal{W}_{v_i}$ **do**
2: $\quad$ **for each** $u_k \in \mathcal{W}_{v_i}[j - w : j + w]$ **do**
3: $\quad\quad J(\Phi) = -\log \Pr(u_k \mid \Phi(v_j))$
4: $\quad\quad \Phi = \Phi - \alpha * \frac{\partial J}{\partial \Phi}$
5: $\quad$ **end for**
6: **end for**

$$\Pr\left(\{v_{i-w}, \cdots, v_{i+w}\} \setminus v_i \mid \Phi(v_i)\right) \underset{\text{independence assumption}}{=} \prod_{\substack{j=i-w \\ j \neq i}}^{i+w} \Pr(v_j | \Phi(v_i))$$

Hierarchical Softmax



$$\Pr(u_k \mid \Phi(v_j)) = \prod_{l=1}^{\lceil \log |V| \rceil} \Pr(b_l \mid \Phi(v_j))$$

path to $u_k \leftarrow (b_0 = \text{root}, b_1, \ldots, b_{\lceil \log |V| \rceil} = u_k)$

$$\Pr(b_l \mid \Phi(v_j) = 1/(1 + e^{-\Phi(v_j) \cdot \Psi(b_l)})$$

sigmoid (binary classifier)

$\Psi(b_\ell) \rightarrow$ representation assigned to b_ℓ

Huffman Coding

assign shorter paths to the frequent vertices in the random walk

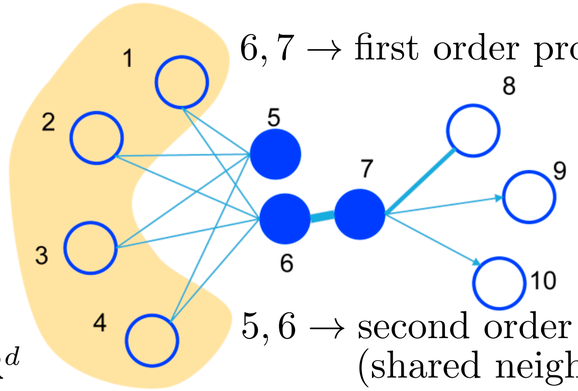
$\theta = \{\Phi, \Psi\}$

Perozzi, Bryan, Rami Al-Rfou, and Steven Skiena. "Deepwalk: Online learning of social representations." *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining*. 2014.

LINE: Large-scale Information Network Embedding

YouTube Video

– visualization – node classification – link prediction – recommendation
$G = (V, E) \rightarrow$ information network (e.g., language, social and citation networks)
$V \rightarrow$ set of vertices (data objects)
$E \rightarrow$ set of edges
$e = (u, v) \rightarrow$ an edge
$w_{uv} \rightarrow$ weight
$(u, v) = (v, u)$ & $w_{uv} = w_{vu} \implies$ undirected
– directed (e.g., citation networks)
– undirected (e.g., social networks of users in Facebook)
– weighted (e.g., word co-occurrence networks)
Represent each vertex $v \in V$ by a low-dimensional vector in $\mathbb{R}^d$
$f_G : V \rightarrow \mathbb{R}^d, d \ll |V|$



$6, 7 \rightarrow$ first order proximity
$5, 6 \rightarrow$ second order proximity (shared neighbors)

	Language Network	Social Network	
Name	WIKIPEDIA	FLICKR	YOUTUBE
Type	undirected,weighted	undirected,binary	undirected,binary
|V|	1,985,098	1,715,256	1,138,499
|E|	1,000,924,086	22,613,981	2,990,443
Avg. degree	504.22	26.37	5.25
#Labels	7	5	47
#train	70,000	75,958	31,703

Citation Network	
DBLP(AUTHORCITATION)	DBLP(PAPERCITATION)
dircted,weighted	directed,binary
524,061	781,109
20,580,238	4,191,677
78.54	10.73
7	7
20,684	10,398

Results of word analogy on WIKIPEDIA data.

Algorithm	Semantic (%)	Syntactic (%)	Overall (%)	Running time
GF	61.38	44.08	51.93	2.96h
DeepWalk	50.79	37.70	43.65	16.64h
SkipGram	69.14	57.94	63.02	2.82h
LINE-SGD(1st)	9.72	7.48	8.50	3.83h
LINE-SGD(2nd)	20.42	9.56	14.49	3.94h
LINE(1st)	58.08	49.42	53.35	2.44h
LINE(2nd)	**73.79**	**59.72**	**66.10**	2.55h

First-order proximity
$(v_i, v_j) \rightarrow$ undirected edge
$p_1(v_i, v_j) \rightarrow$ joint probability btw vertices v_i & v_j
$p_1(v_i, v_j) = \sigma(u_i^T u_j)$
$u_i \in \mathbb{R}^d \rightarrow$ vector representation of vertex v_i
$p_1 \rightarrow$ distribution over $V \times V$
$\hat{p}_1 \rightarrow$ empirical counterpart of p_1

$$\hat{p}_1(v_i, v_j) = \frac{w_{ij}}{W}, \quad W = \sum_{(v_i, v_j) \in E} w_{v_i v_j}$$

$O_1 = d(\hat{p}_1, p_1) \rightarrow$ e.g., KL-divergence

$$O_1 = -\sum_{(v_i, v_j) \in E} w_{v_i v_j} \log p_1(v_i, v_j)$$

ignoring the constants

Second-order proximity
Each vertex plays two roles:
– the vertex itself: u_i
– "context" of other vertices: $\overline{u}_i$

$$p_2(v_j|v_i) = \frac{\exp(\overline{u}_j^T u_i)}{\sum_{k=1}^{V} \exp(\overline{u}_k^T u_i)}$$

probability of context v_j generated by vertex v_i

$$O_2 = \sum_{v_i \in V} \lambda_i d(\hat{p}_2(\cdot|v_i), p_2(\cdot|v_i))$$

$\lambda_i \rightarrow$ importane of vertex v_i (e.g., degree)

$$\hat{p}_2(v_j|v_i) = \frac{w_{ij}}{d_i} \rightarrow \text{out-degree of vertex } v_i$$

$$d_i = \sum_{v_k \in N(v_i)} w_{v_i v_k}$$

$$O_2 = -\sum_{(v_i, v_j) \in E} w_{v_i v_j} \log p_2(v_j|v_i) \rightarrow \text{setting } \lambda_i = d_i$$

ignoring the constants

$$\log p_2(v_j|v_i) \approx \log \sigma(\overline{u}_j^T u_i) + \sum_{k=1}^{K} \mathbb{E}_{v_k \sim P(v_k)} \log \sigma(-\overline{u}_k^T u_i)$$

$K \rightarrow$ number of negative samples (i.e., edges)
$P(v) \propto d_v^{3/4}$
$d_v \rightarrow$ out-degree of vertex v
Sample edges according to their weights $(w_1, \ldots, w_{|E|})$

Tang, Jian, et al. "Line: Large-scale information network embedding." *Proceedings of the 24th international conference on world wide web*. 2015.

node2vec: Scalable Feature Learning for Networks

YouTube Video

$G = (V, E) \rightarrow$ a given network

$f : V \rightarrow \mathbb{R}^d$

$\hookrightarrow$ a matrix of size $|V| \times d$

$u \in V \rightarrow$ source node

$N_S(u) \subset V \rightarrow$ network neighborhood of node u

$S \rightarrow$ neighborhood sampling strategy

Skip-gram

$$\max_f \sum_{u \in V} \log \Pr(N_S(u)|f(u))$$

Conditional Independence

$$\Pr(N_S(u)|f(u)) = \prod_{n_i \in N_S(u)} \Pr(n_i|f(u))$$

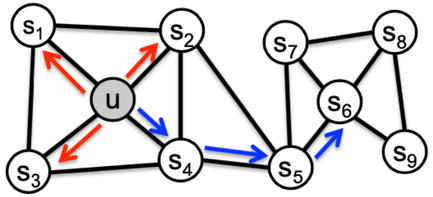
Symmetry in feature space

$$\Pr(n_i|f(u)) = \frac{\exp(f(n_i) \cdot f(u))}{\sum_{v \in V} \exp(f(v) \cdot f(u))}$$

$$\max_f \sum_{u \in V} [-\log Z_u + \sum_{n_i \in N_S(u)} f(n_i) \cdot f(u)]$$

$$Z_u = \sum_{v \in V} \exp(f(u) \cdot f(v)) \rightarrow \text{expensive to compute}$$

approximate using negative sampling



Breadth-First Sampling

→BFS

$k = 3 \rightarrow$ neighborhood size

→DFS

Depth-First Sampling

Random Walk

$c_i \rightarrow i$-th node in the walk

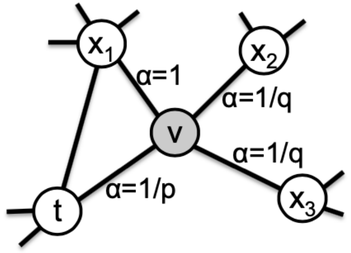
$c_0 = u$

$$p(c_i = x|c_{i-1} = v) = \begin{cases} \frac{1}{z}\pi_{vx} & \text{if } (v, x) \in E \\ 0 & \text{otherwise} \end{cases}$$

$z \rightarrow$ normalization constant

$\pi_{vx} \rightarrow$ unnormalized transition probability btw nodes v & x

$w_{vx}\ (= 1) \rightarrow$ edge weights



$$\pi_{vx} = \alpha_{pq}(t, x) \cdot w_{vx}$$

$$\alpha_{pq}(t, x) = \begin{cases} \frac{1}{p} & \text{if } d_{tx} = 0 \\ 1 & \text{if } d_{tx} = 1 \\ \frac{1}{q} & \text{if } d_{tx} = 2 \end{cases}$$

A walk that just transitioned from t to v and is now evaluating its next step out of node v.

$d_{tx} \rightarrow$ shortest path distance between nodes t and x

$$p > q \ \&\ p > 1 \implies \frac{1}{p} < 1 \ \&\ \frac{1}{p} < \frac{1}{q} \implies$$

lower weight on the prob. of returning to t

$$p < q \ \&\ p < 1 \implies \frac{1}{p} > 1 \ \&\ \frac{1}{p} > \frac{1}{q} \implies$$

higher weight on the prob. of returning to t

$p \rightarrow$ return parameter

$q > 1 \implies$ local

$q < 1 \implies$ global $\implies$ q is the in-out parameter

(approximately) interpolate between BFS & DFS

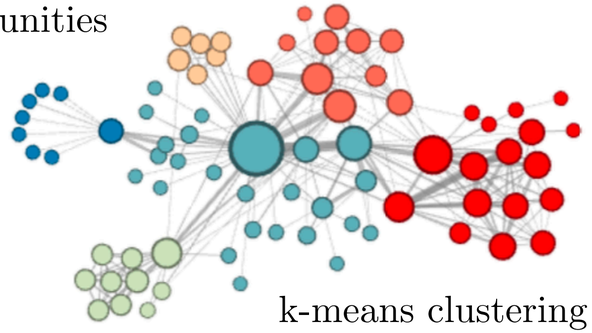
Edge Features

Operator	Symbol	Definition
Average	$\boxplus$	$[f(u) \boxplus f(v)]_i = \frac{f_i(u)+f_i(v)}{2}$
Hadamard	$\boxdot$	$[f(u) \boxdot f(v)]_i = f_i(u) * f_i(v)$
Weighted-L1	$\|\cdot\|_{\bar{1}}$	$\|f(u) \cdot f(v)\|_{\bar{1}i} = \|f_i(u) - f_i(v)\|$
Weighted-L2	$\|\cdot\|_{\bar{2}}$	$\|f(u) \cdot f(v)\|_{\bar{2}i} = \|f_i(u) - f_i(v)\|^2$

network communities

$p = 1, q = 2$

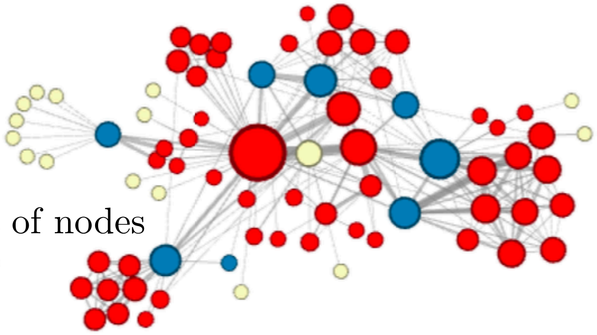
Nodes correspond to characters in the novel Les Misérables and edges connect coappearing characters. The network has 77 nodes and 254 edges.



k-means clustering

structural roles of nodes

$p = 1, q = 0.5$



Grover, Aditya, and Jure Leskovec. "node2vec: Scalable feature learning for networks." Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining. 2016.

Semi-Supervised Classification with Graph Convolutional Networks

Boulder

YouTube Playlist

Consider the problem of classifying nodes (such as documents) in a graph (such as a citation network), where labels are only available for a small subset of nodes.

$\mathcal{G} = (\mathcal{V}, \mathcal{E})$ → undirected graph

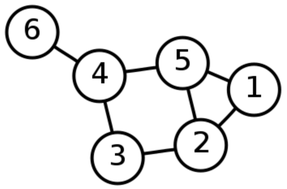
$\mathcal{V} = \{v_i : i = 1, \ldots, N\}$ → nodes

$(v_i, v_j) \in \mathcal{E}$ → edges

$A \in \mathbb{R}^{N \times N}$ → adjacency matrix (binary or weighted)

$D_{ii} = \sum_j A_{ij}$ → degree matrix

$\Delta = D - A$ → unnormalized graph Laplacian



$$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$$

https://en.wikipedia.org/wiki/Laplacian_matrix#Interpretation_as_the_discrete_Laplace_operator

$\mathcal{L} = \mathcal{L}_0 + \lambda \mathcal{L}_{\text{reg}}$ (supervised loss)

$$\mathcal{L}_{\text{reg}} = \sum_{i,j} A_{ij} \|f(X_i) - f(X_j)\|^2 = f(X)^T \Delta f(X)$$ (neural network)

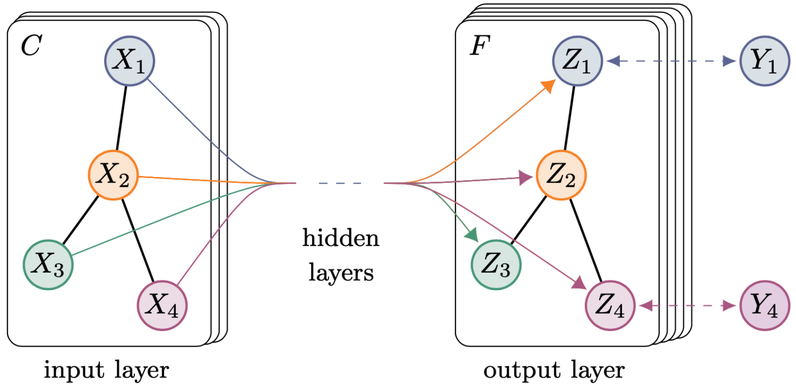
X → matrix of node feature vectors X_i

Convolutions on Graphs

$\tilde{A} = A + I \qquad \tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$

Motivated by a first-order approximation of localized spectral filters on graphs (see the paper)

$H^{\ell+1} = \sigma(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{\ell} W^{\ell}) \qquad H^0 = X \qquad H^{\ell} \in \mathbb{R}^{N \times D}$



Graph Convolutional Network

$\hat{A} = \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}}$ → pre-processing step

$Z = f(X, A) = \text{softmax}\Big(\hat{A}\ \text{ReLU}\Big(\hat{A} X W^{(0)}\Big) W^{(1)}\Big)$

$W^{(0)} \in \mathbb{R}^{C \times H}$

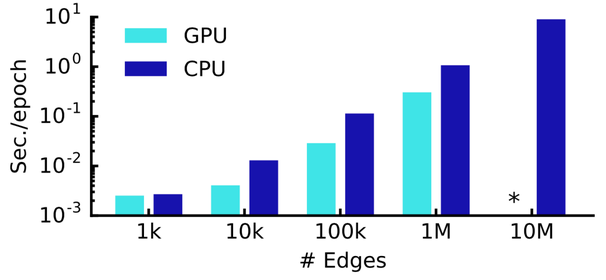
$W^{(1)} \in \mathbb{R}^{H \times F}$

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

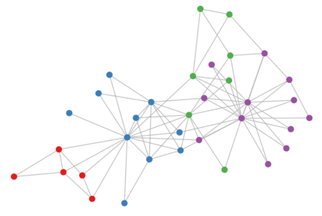
cross-entropy error

set of node indices that have labels

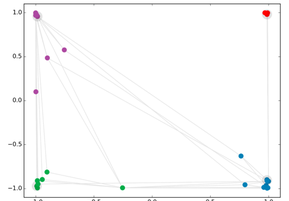
Drawback: batch gradient descent



Wall-clock time per epoch for random graphs. (*) indicates out-of-memory error.



(a) Karate club network

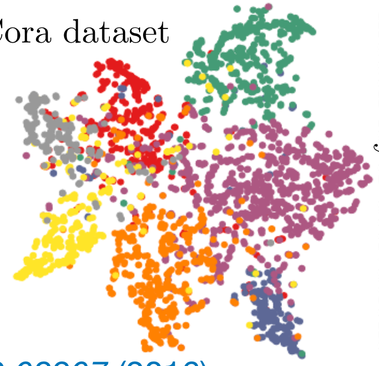


(f) Iteration 300

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

Method	Citeseer	Cora	Pubmed	NELL
ManiReg [3]	60.1	59.5	70.7	21.8
SemiEmb [28]	59.6	59.0	71.1	26.7
LP [32]	45.3	68.0	63.0	26.5
DeepWalk [22]	43.2	67.2	65.3	58.1
ICA [18]	69.1	75.1	73.9	23.1
Planetoid* [29]	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

Cora dataset



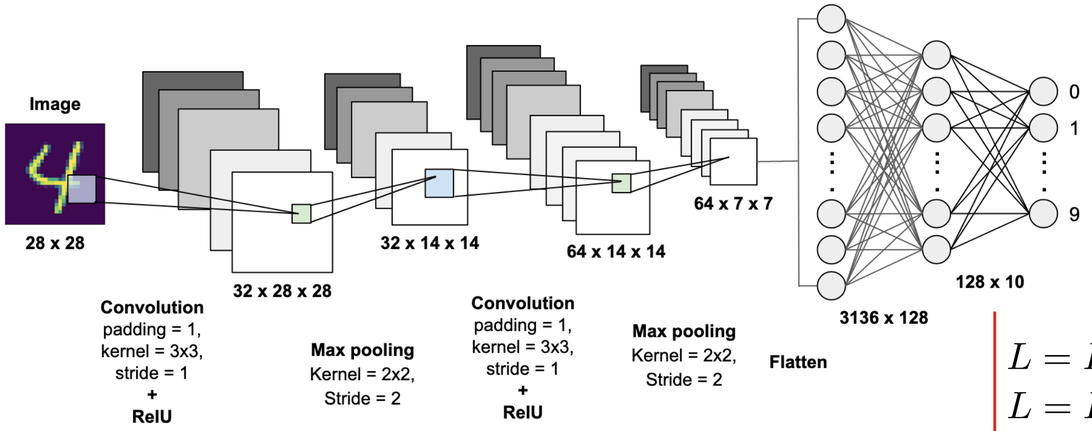
hidden layer activations

Kipf, Thomas N., and Max Welling. "Semi-supervised classification with graph convolutional networks." *arXiv preprint arXiv:1609.02907* (2016).

Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering

Boulder

YouTube Video



Regular grids (e.g., image, video and speech)

Irregular domains (e.g., social networks, brain connectomes or words' embedding) represented by graphs

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

$\mathcal{V} \rightarrow$ finite set of $|\mathcal{V}| = n$ vertices

$\mathcal{E} \rightarrow$ set of edges

$W \in \mathbb{R}^{n \times n} \rightarrow$ weighted adjacency matrix (encoding the connection weight btw two vertices)

Example (image): 8-NN graph of the 2D grid $n = |\mathcal{V}| = 976$ ($28^2 = 784$ pixels plus 192 fake nodes)

$|\mathcal{E}| = 3198$

$W_{ij} = \exp\left(-\frac{\|z_i - z_j\|_2^2}{\sigma^2}\right)$ z_i is the 2D coordinate of pixel i

$x : \mathcal{V} \rightarrow \mathbb{R}$

↳ a signal on the nodes of the graph (e.g., an image)

$x \in \mathbb{R}^n, x_i \rightarrow$ value of x at node i

– user data on social networks

– gene data on biological regulatory networks

– log data on telecommunication networks

– text documents on word embeddings

Graph Laplacian

$D \in \mathbb{R}^{n \times n} \rightarrow$ diagonal degree matrix

$D_{ii} = \sum_j W_{ij}$

$L = D - W \rightarrow$ combinatorial definition

$L = I_n - D^{-\frac{1}{2}} W D^{-\frac{1}{2}} \rightarrow$ normalized definition

$L \rightarrow$ real symmetric positive semidefinite matrix

$\{u_l \in \mathbb{R}^n\}_{l=1}^{n-1} \rightarrow$ complete set of orthonormal eigenvectors

Graph Fourier Modes

$\{\lambda_l\}_{l=1}^{n-1} \rightarrow$ corresponding ordered real nonnegative eigenvalues

Frequencies of the Graph

$U = [u_0, \ldots, u_{n-1}] \in \mathbb{R}^{n \times n} \rightarrow$ Fourier Basis

$\Lambda = \mathrm{diag}([\lambda_0, \ldots, \lambda_{n-1}]) \in \mathbb{R}^{n \times n}$

$L = U \Lambda U^T \rightarrow$ diagonalized

$\hat{x} = U^T x \rightarrow$ Fourier Transform

$x = U\hat{x} \rightarrow$ Inverse Fourier Transform

$*_{\mathcal{G}} \rightarrow$ graph convolution

$x *_{\mathcal{G}} y := U((U^T x) \odot (U^T y))$

Spectral Filtering

$g_\theta(L)x = g_\theta(U \Lambda U^T)x = U g_\theta(\Lambda) U^T x$

↳ signal x filtered by g_θ

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

– non-localized in space

– learning complexity $\mathcal{O}(n)$

Polynomial Parametrization

Chebyshev Polynomials

$T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$

$T_0(x) = 1, T_1(x) = x$

$g_\theta(\Lambda) = \sum_{k=0}^{K-1} \theta_k T_k(\tilde{\Lambda}), \tilde{\Lambda} = \frac{2\Lambda}{\lambda_{\max}} - I_n$

Model	Accuracy
Classical CNN	99.33
Proposed graph CNN	99.14

The proposed spectral filters are provable to be strictly localized in a ball of radius K, i.e. K hops from the central vertex.

$\theta \in \mathbb{R}^K$

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

$\tilde{L} = 2L/\lambda_{max} - I_n$

$\bar{x}_k = T_k(\tilde{L})x$

$\bar{x}_k = 2\tilde{L}\bar{x}_{k-1} - \bar{x}_{k-2}$

$\bar{x}_0 = x$

$\bar{x}_1 = \tilde{L}x$

Graph Coarsening and Pooling (see the paper)

$\mathcal{O}(K|\mathcal{E}|)$ operations

Defferrard, Michaël, Xavier Bresson, and Pierre Vandergheynst. "Convolutional neural networks on graphs with fast localized spectral filtering." *arXiv preprint arXiv:1606.09375* (2016).

Inductive Representation Learning on Large Graphs

YouTube Video

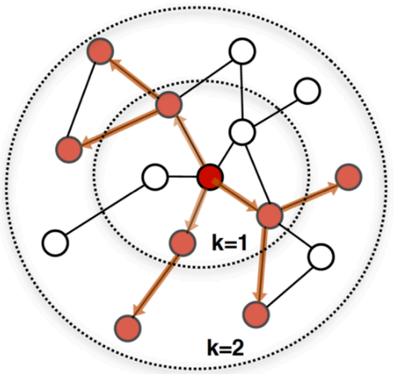
Large Graphs: Social or Biological Networks
– content recommendation
– identifying protein functions
Transductive: Single Fixed Graph
Inductive: Dynamic Graph
– Citation & Reddit post data
– Protein-protein interaction
Low-dimensional vector embeddings of nodes in large graphs
– node classification
– clustering
– link prediction
Nodes: posts on Reddit or users and videos on Youtube
GraphSAGE: SAmple & aggreGatE
Node features: – text attributes
– node profile information
– node degrees
– citation data with text attributes
– biological data with functional/molecular markers

Mean aggregator → Similar to GCN

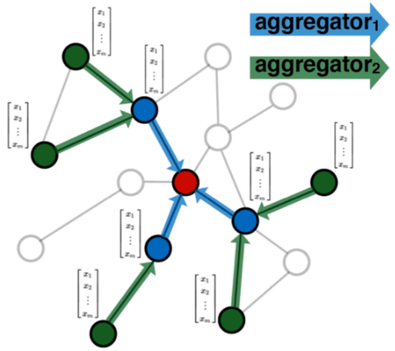
$$\mathbf{h}_v^k \leftarrow \sigma(\mathbf{W} \cdot \text{MEAN}(\{\mathbf{h}_v^{k-1}\} \cup \{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}(v)\})$$

Pooling aggregator

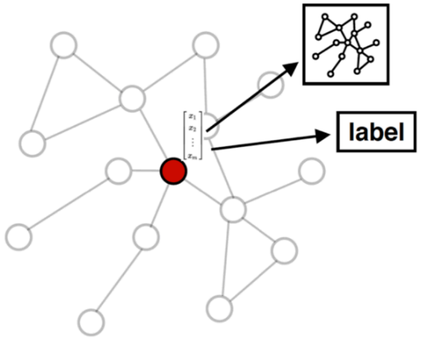
$$\text{AGGREGATE}_k^{\text{pool}} = \max(\{\sigma\left(\mathbf{W}_{\text{pool}}\mathbf{h}_{u_i}^k + \mathbf{b}\right), \forall u_i \in \mathcal{N}(v)\})$$



1. Sample neighborhood



2. Aggregate feature information from neighbors



3. Predict graph context and label using aggregated information

(i) classifying academic papers into different subjects using the Web of Science citation dataset
(ii) classifying Reddit posts as belonging to different communities, and
(iii) classifying protein functions across various biological protein-protein interaction (PPI) graphs.

Algorithm 1: GraphSAGE embedding generation (i.e., forward propagation) algorithm

Input : Graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$; input features $\{\mathbf{x}_v, \forall v \in \mathcal{V}\}$; depth K; weight matrices $\mathbf{W}^k, \forall k \in \{1, ..., K\}$; non-linearity σ; differentiable aggregator functions $\text{AGGREGATE}_k, \forall k \in \{1, ..., K\}$; neighborhood function $\mathcal{N} : v \rightarrow 2^{\mathcal{V}}$
Output : Vector representations $\mathbf{z}_v$ for all $v \in \mathcal{V}$

$\mathbf{h}_v^0 \leftarrow \mathbf{x}_v, \forall v \in \mathcal{V}$;
for $k = 1...K$ **do**
  for $v \in \mathcal{V}$ **do**
    $\mathbf{h}_{\mathcal{N}(v)}^k \leftarrow \text{AGGREGATE}_k(\{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}(v)\})$;
    $\mathbf{h}_v^k \leftarrow \sigma\left(\mathbf{W}^k \cdot \text{CONCAT}(\mathbf{h}_v^{k-1}, \mathbf{h}_{\mathcal{N}(v)}^k)\right)$
  end
  $\mathbf{h}_v^k \leftarrow \mathbf{h}_v^k / \|\mathbf{h}_v^k\|_2, \forall v \in \mathcal{V}$
end
$\mathbf{z}_v \leftarrow \mathbf{h}_v^K, \forall v \in \mathcal{V}$

$$J_{\mathcal{G}}(\mathbf{z}_u) = -\log\left(\sigma(\mathbf{z}_u^\top \mathbf{z}_v)\right) - Q \cdot \mathbb{E}_{v_n \sim P_n(v)} \log\left(\sigma(-\mathbf{z}_u^\top \mathbf{z}_{v_n})\right)$$

Encourages nearby nodes to have similar representations, while enforcing that the representations of disparate nodes are highly distinct

$v \rightarrow$ a node that co-occurs near u on a fixed-length random walk
$P_n \rightarrow$ negative sampling distribution
$Q \rightarrow$ number of negative samples

Hamilton, Will, Zhitao Ying, and Jure Leskovec. "Inductive representation learning on large graphs." *Advances in neural information processing systems*. 2017.

Graph Attention Networks

YouTube Video

GATs: Graph ATtention networks
- Cora
- Citeseer
- Pubmed

} citation

- Protein-protein interaction

Graphs: 3D meshes, social networks, telecommunication networks, biological networks or brain connectomes

Graph Attentional Layer

$h = \{h_1, h_2, \ldots, h_N\}, h_i \in \mathbb{R}^F$

input (a set of node features)

$N \rightarrow$ number of nodes

$F \rightarrow$ number of features

$h' = \{h'_1, h'_2, \ldots, h'_N\}, h'_i \in \mathbb{R}^{F'}$

output

$W \in \mathbb{R}^{F' \times F} \rightarrow$ weight matrix

Self-attention

$a : \mathbb{R}^{F'} \times \mathbb{R}^{F'} \rightarrow \mathbb{R}$

$e_{ij} = a(Wh_i, Wh_j) \rightarrow$ attention coefficient (importance of node j's features to node i)

Masked attention

$\mathcal{N}_i \rightarrow$ some neighborhood of node i in the graph (first-order neighbors of i, including i)

$$\alpha_{ij} = \text{softmax}_j(e_{ij}) = \frac{\exp(e_{ij})}{\sum_{k \in \mathcal{N}_i} \exp(e_{ik})}$$

$$a(x, y) = \text{LeakyReLU}_{\alpha=2}(a^T [x \| y]), a \in \mathbb{R}^{2F'}$$

concatenation

$$h'_i = \sigma\left(\sum_{j \in \mathcal{N}_i} \alpha_{ij} W h_j\right)$$

Multi-head Attention (K heads)

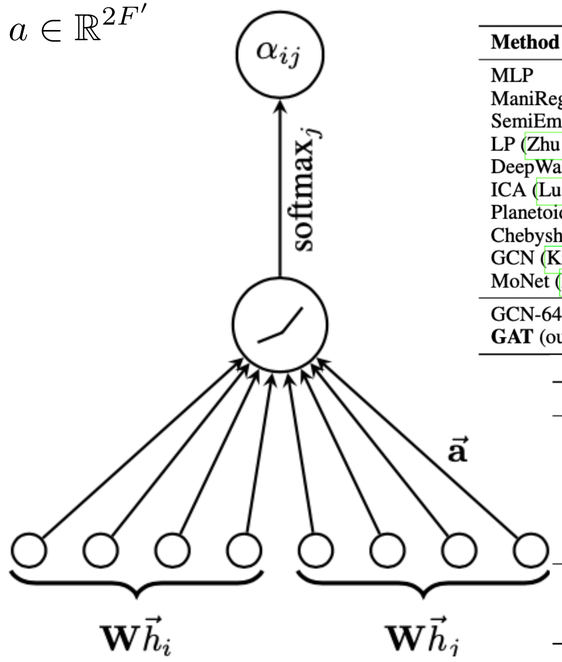
$$h'_i = \Big\Vert_{k=1}^{K} \sigma\left(\sum_{j \in \mathcal{N}_i} \alpha_{ij}^k W^k h_j\right)$$

concatenation

$KF' \rightarrow$ features

Final Prediction Layer

$$h'_i = \sigma\left(\frac{1}{K} \sum_{k=1}^{K} \sum_{j \in \mathcal{N}_i} \alpha_{ij}^k W^k h_j\right)$$



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 ± 0.5%	—	78.8 ± 0.3%
GCN-64*	81.4 ± 0.5%	70.9 ± 0.5%	**79.0** ± 0.3%
GAT (ours)	**83.0** ± 0.7%	**72.5** ± 0.7%	**79.0** ± 0.3%

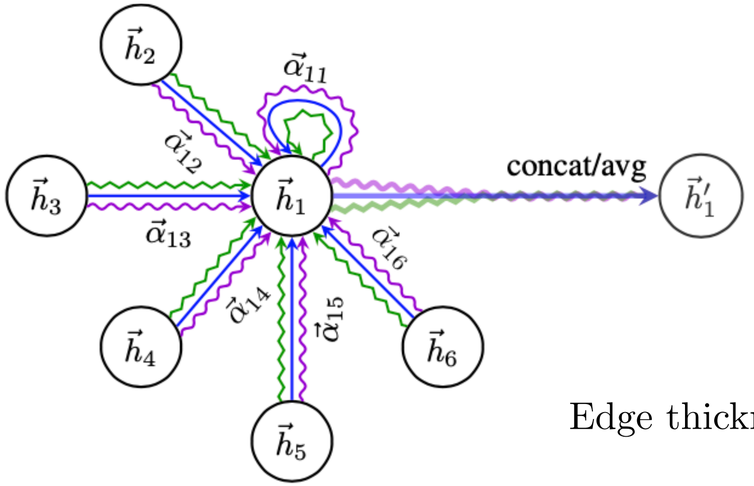
accuracies

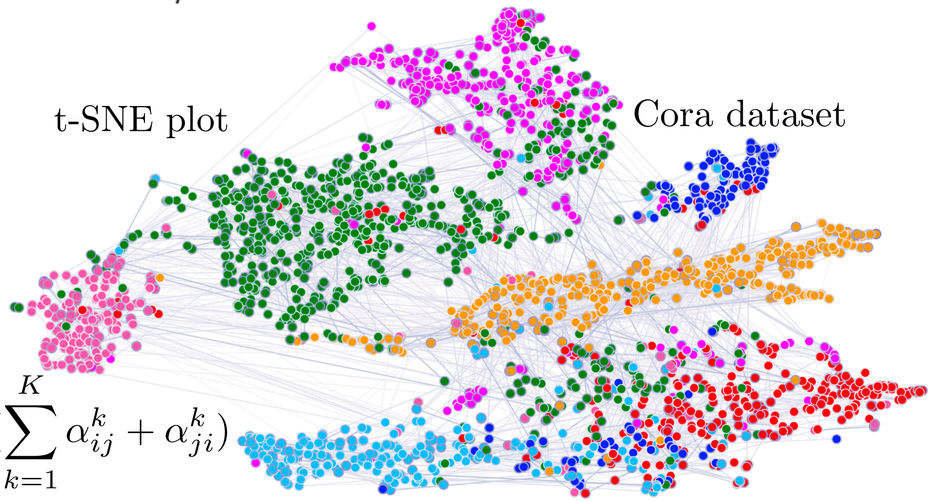
Inductive

Method	PPI
Random	0.396
MLP	0.422
GraphSAGE-GCN (Hamilton et al., 2017)	0.500
GraphSAGE-mean (Hamilton et al., 2017)	0.598
GraphSAGE-LSTM (Hamilton et al., 2017)	0.612
GraphSAGE-pool (Hamilton et al., 2017)	0.600
GraphSAGE*	0.768
Const-GAT (ours)	0.934 ± 0.006
GAT (ours)	**0.973** ± 0.002

F1 scores

$$2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$





Edge thickness: $\left(\sum_{k=1}^{K} \alpha_{ij}^k + \alpha_{ji}^k\right)$

Veličković, Petar, et al. "Graph attention networks." *arXiv preprint arXiv:1710.10903* (2017).

How Powerful Are Graph Neural Networks?

YouTube Video

$G = (V, E) \rightarrow$ graph
$X_v \rightarrow$ node feature vector for $v \in V$

Node Classification

$y_v \rightarrow$ associated label to node $v \in V$
$h_v \rightarrow$ representation vector of $v \in V$
$y_v = f(h_v)$

Graph Classification

$\{G_1, \ldots, G_N\} \subset \mathcal{G} \rightarrow$ set of graphs
$\{y_1, \ldots, y_N\} \subset \mathcal{Y} \rightarrow$ set of labels
$h_G \rightarrow$ representation vector
$y_G = g(h_G) \rightarrow$ predicted label of an entire graph

Graph Neural Networks (GNNs)

$k \rightarrow k$-th layer of a GNN (k-th iteration)

$$a_v^{(k)} = \text{AGGREGATE}^{(k)}(\{h_u^{(k-1)} : u \in \mathcal{N}(v)\})$$

(set of nodes adjacent to v)

$$h_v^{(k)} = \text{COMBINE}^{(k)}(h_v^{(k-1)}, a_v^{(k)})$$

$$h_v^{(0)} = X_v$$

Graph Classification

$$h_G = \text{READOUT}(\{h_v^K : v \in G\})$$

summation or group-level pooling function

GraphSage

$$a_v^{(k)} = \text{MAX}(\{\text{ReLU}(W h_u^{(k-1)}), \forall u \in \mathcal{N}(v)\}) \rightarrow \text{aggregate}$$

$$W[h_v^{(k-1)}, a_v^{(k)}] \rightarrow \text{combine}$$

Graph Convolutional Network (GCN)

$$h_v^{(k)} = \text{ReLU}(W \ \text{MEAN}(\{h_u^{k-1}, \forall u \in \mathcal{N}(v) \cup \{v\}\}))$$

(aggregate and combine)

Graph Isomorphism Network (GIN)

$$h_v^{(k)} = \text{MLP}^{(k)}\left(\left(1 + \epsilon^{(k)}\right) \cdot h_v^{(k-1)} + \sum_{u \in \mathcal{N}(v)} h_u^{(k-1)}\right)$$

$$h_G = \text{CONCAT}\left(\text{READOUT}\left(\left\{h_v^{(k)} | v \in G\right\}\right) \mid k = 0, 1, \ldots, K\right)$$

Discriminative and representational power of GIN is equal to the power of the Weisfeiler-Lehman test.

Weisfeiler-Lehman (WL) Test

Graph isomorphism problem: Are two graphs topologically identical?

The WL test iteratively (1) aggregates the labels of nodes and their neighborhoods, and (2) hashes the aggregated labels into unique new labels. The algorithm decides that two graphs are non-isomorphic if at some iteration the labels of the nodes between the two graphs differ.

Proof (Sketch)

– GNNs are at most as powerful as the WL test in distinguishing graph structures

Let G_1 and G_2 be any two non-isomorphic graphs. If a graph neural network $\mathcal{A} : \mathcal{G} \rightarrow \mathbb{R}^d$ maps G_1 and G_2 to different embeddings, the Weisfeiler-Lehman graph isomorphism test also decides G_1 and G_2 are not isomorphic.

– Under some mild conditions on the neighbor aggregation and graph readout functions, the resulting GNN is as powerful as the WL test.

a) $\mathcal{A}$ aggregates and updates node features iteratively with

$$h_v^{(k)} = \phi\left(h_v^{(k-1)}, f\left(\left\{h_u^{(k-1)} : u \in \mathcal{N}(v)\right\}\right)\right),$$

where the functions f, which operates on multisets, and ϕ are injective.

b) $\mathcal{A}$'s graph-level readout, which operates on the multiset of node features $\left\{h_v^{(k)}\right\}$, is injective.

Xu, Keyulu, et al. "How powerful are graph neural networks?." *arXiv preprint arXiv:1810.00826* (2018).

Boulder

Questions?

YouTube Playlist