node2vec: Scalable Feature Learning for Networks

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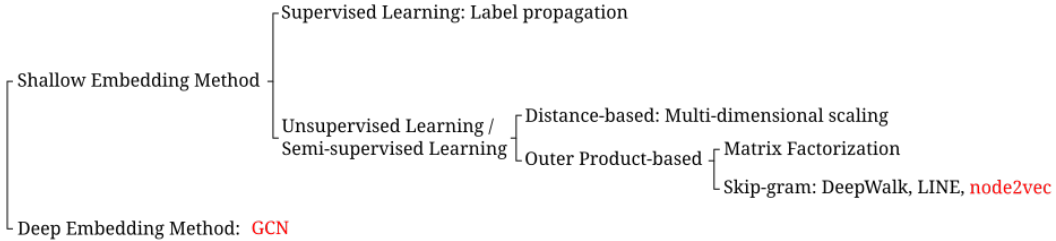
Introduction to Graph Embeddings

- Represent graph-structured data.
- Applications:
  Social network analysis, recommender systems, molecular structure modelling, etc.
- Challenge: Limitations of traditional methods.
- Development of techniques specially for graph representations.

Related Work

A taxonomy of graph embedding techniques[1].



[1] Kevin P. Murphy. *Probabilistic Machine Learning: An Introduction*. Adaptive Computation and Machine Learning series. MIT Press, 2022. ISBN: 9780262046824.

Feature Learning Framework

- Goal: Given a network $G = (V, E)$, find a projection $f : V \rightarrow R^d$.
- Generate a d-dimesion vector representation for each node.
- f can be formulated as a matrix of size $|V| \cdot d$.

Feature Learning Framework

Extending skip gram architecture to networks.

Formulate feature learning in networks as a maximum likelihood optimization problem:

$$\max_{f} \sum_{u \in V} \log Pr\left(N_S\left(u\right) | f(u)\right)$$

$N_S\left(a\right)$ is the network neighborhood set generated by neighborhood sampling strategy S for node a.

Important: $N_S\left(a\right)$ isn't equavalent to direct local neighborhood.

For NLP: This is a [feature learning framework social network].

$$Pr(\{\text{"feature"},\text{"learning"},\text{"social"},\text{"network"}\}|\text{"framework"})$$

For Graph:

$$N_S\left(a\right) = \{b, c, d, e\}$$
$$Pr\left(\{b, c, d, e\} | a\right) = Pr\left(N_s\left(a\right) | a\right)$$

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Two problems to be solved:

1. How to define $N_S\left(a\right)$?
2. How to compute $Pr\left(N_S\left(a\right) | a\right)$?

Maximum Likehood Optimization

Formulate feature learning in networks as a maximum likelihood optimization problem:

$$\max_{f} \sum_{u \in V} \log Pr\left(N_S\left(u\right) | f(u)\right)$$

Two standard assumptions:

1. Conditional independence:

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

2. Symmetry in feature space:

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

Maximum Likehood Optimization

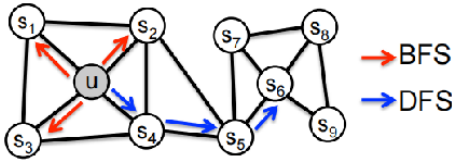
Finally, the optimization problem is converted into the form of:

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

Use gradient decent stochastic to obtain projection f.

Network Neighborhood Sampling Strategy

Use classic search strategies:
Breadth-first Sampling (BFS) and Depth-first Sampling (DFS).



There are two kinds of similarities:

1. homophily (such as u and s_1)
2. structural equivalence (such as u and s_6)

DFS tends to discover homophily, BFS tends to discover structural equivalence.

How to discover both kinds of similarities?

Network Neighborhood Sampling Strategy

Use basic random walk to discover both homophily and structural equalvalence similarities.

Basic random walk with length l from source node u:

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

c_i: the i-th node in the walk.

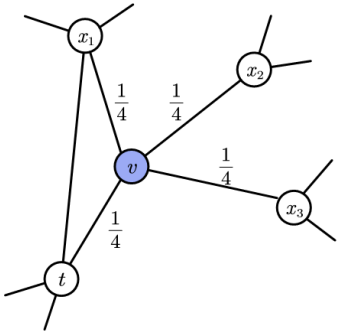
v: current node.

π_{vx}: unnormalized transition probability.

Z: normalization constant.

Network Neighborhood Sampling Strategy

π_{vx}: Often set $\pi_{vx} = w_{vx}$ in weighted graphs.
In unweighted graph: $\pi_{vx} = 1$.



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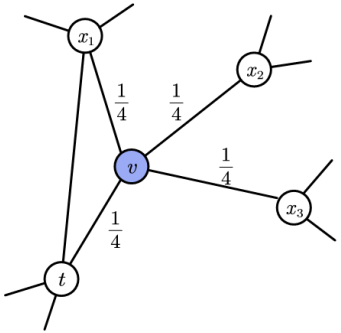


Ramdom walk can combine features of DFS and BFS, and discovery both two kinds of similarities.

Still not enough:
It's hard for us to guide and control the walking process.

Network Neighborhood Sampling Strategy

Use the second order bias random walk to get control of the walking process.

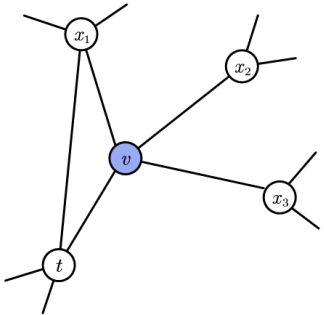
$$\pi_{vx} = \alpha_{pq}(t,x) \cdot w_{vx}$$

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

v: current node.

t: last node in the walk.

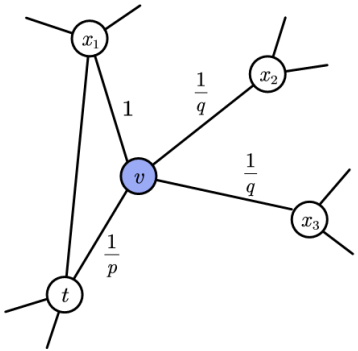
x: next node to be chosen.



Network Neighborhood Sampling Strategy

p: return parameter.

q: in-out parameter.



p :

- when set a high value: less likely to sample an already visited node.
- when set a low value: likely to step back, then walk locally near the source node u.

q :

- when set a high value: biased towards nodes close to t, act more similarly to BFS.
- when set a low value: biased towards nodes distant to t, act more similarly to DFS.

Learning Edge Features

We have found a projection $f : V \rightarrow R^d$ with node2vec, which allocates each node vector embedding representation.

These embedding vectors can be used in node-related downstream tasks.

But how to learn edge features and deal with edge-related downstream tasks?

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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	$\|\cdot\|_{\bar{2}}$	$\|f(u) \cdot f(v)\|_{\bar{2}_i} = \|f_i(u) - f_i(v)\|^2$

Given projection f obtained by node2vec and two nodes u, v along with edge (u, v), apply the binary operator on $f(u)$ and $f(v)$ to generate the representation $g(u, v)$, where $g : V \times V \to R^{d'}$.

Experiment 1: Multi-label Classification

- Task description
  - Labels from a finite set $\mathcal{L}$
  - Training: A fraction of nodes and all their labels.
  - Predict the labels for the remaining nodes.
- Data

Dataset	Nodes	Edges	Labels
BlogCatalog	10,312	333,983	39
Protein-Protein Interactions (PPI)	3,890	76,584	50
Wikipedia	4,777	184,812	40

Experiment 1: Multi-label Classification

- Results

Algorithm	**Dataset**		
	BlogCatalog	PPI	Wikipedia
Spectral Clustering	0.0405	0.0681	0.0395
DeepWalk	0.2110	0.1768	0.1274
LINE	0.0784	0.1447	0.1164
node2vc	**0.2581**	**0.1791**	**0.1552**
node2vec settings (p, q)	0.25, 0.25	4, 1	4, 0.5
Gain of node2vec [%]	**22.3**	**1.3**	**21.8**

Experiment 2: Link Prediction

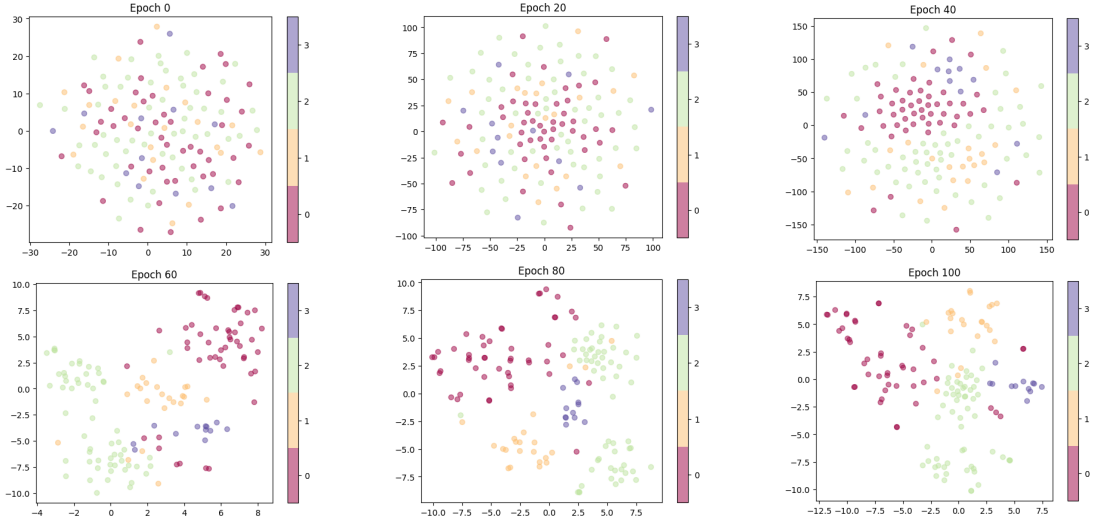
- Task description
  - A network with a fraction of edges removed.
  - Predict these missing edges.
- Data

Dataset	Nodes	Edges
Facebook	4,039	88,234
Protein-Protein Interactions (PPI)	19,706	390,633
arXiv ASTRO-PH	18,722	198,110

Experiment 2: Link Prediction

- Results

Algorithm	**Dataset**		
	Facebook	PPI	arXiv
Common Neighbors	0.8100	0.7142	0.8153
Jaccard's Coefficient	0.8880	0.7018	0.8067
Adamic-Adar	0.8289	0.7126	0.8315
Pref. Attachment	0.7137	0.6670	0.6996
Spectral Clustering	0.6192	0.4920	0.5740
DeepWalk	**0.9680**	0.7441	0.9340
LINE	0.9490	0.7249	0.8902
mode2vec	**0.9680**	**0.7719**	**0.9366**



AIFB dataset: Each node has a category label. There are 4 classes in total.

During the training of node2vec, nodes embedding are changed from chaos into order.

Graph Neural Network

Graph Neural Network is a deep learning framework for graph.

General GNN iteration formula:

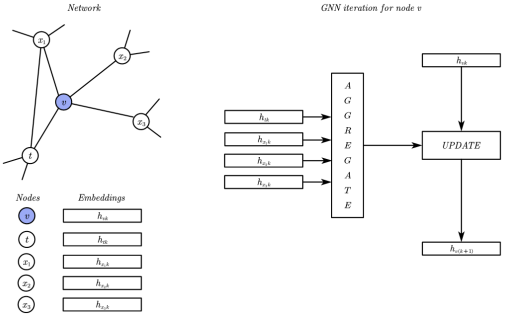
$$h_u^{(k)} = \sigma(W_{\text{self}}^{(k)} h_u^{(k-1)} + W_n^{(k)} \sum_{v \in N(u)} h_v^{(k-1)} + b^{(k)})$$

$h_u^{(k)}$: k-th layer output embedding of node u.

$W^{(k)}$: weights of k-th layer (trainable).

$b^{(k)}$: bias of k-th layer (trainable).

σ: activation function.



Aggregate: To aggregate embeddings of u's neighborhood.

Update: To update u's embeddings using aggregation result and previous u's embeddings.

Graph Neural Network

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Final output embeddings can be used for calculating predictions. Then, we can use these predictions to compute the loss and optimize parameters with back propagation.

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Problem: How to produce h_u^0 for each node?

1. Use one-hot vector for each node.
   - Drawback: The total number of nodes is large. Using one-hot vector for each node will cause the input tensor to be very sparse.

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3. Use a trainable embedding layer to allocate randomly initialized embeddings for each node.
   - Drawback: Randomly initialized embeddings could have negative impact on training process.

Combine node2vec and GNN

node2vec can produce embeddings for each node with graph information.

GNN lacks a good general method to initialize its input nodes' embeddings.

We can use node2vec to produce initial input nodes' embedding for GNN to improve training process of GNN and obtain better performance.

It's a general method because there is no specific requirement of graphs when applying node2vec and GNN.

Proposed Method

Preliminary Results

Future work