Seminar II: Deep Learning-based Natural Language Processing

“node2vec: Scalable Feature Learning for Networks”
Paper review

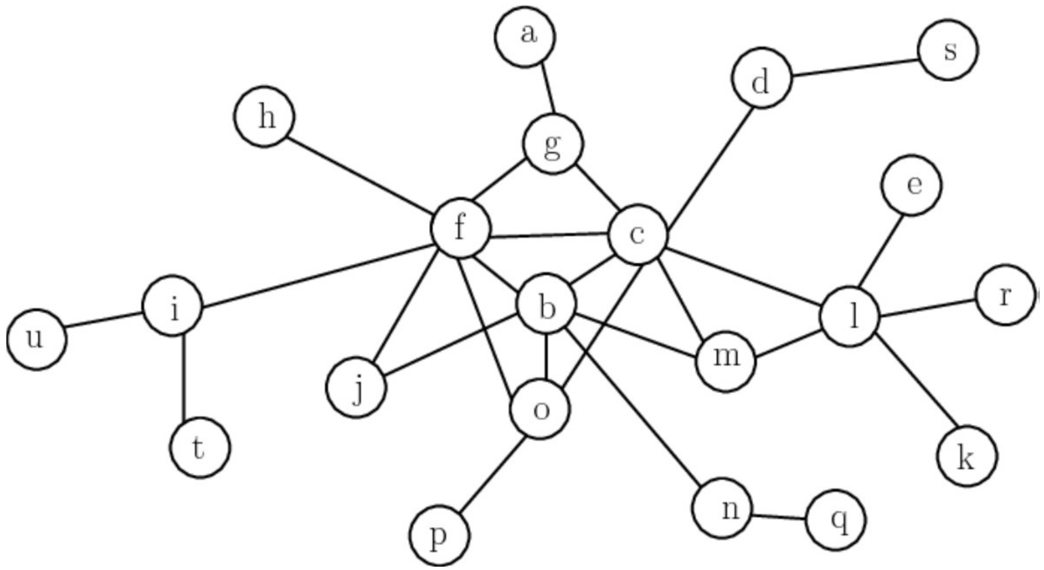
Contents

Introduction. Graphs

Data consist of

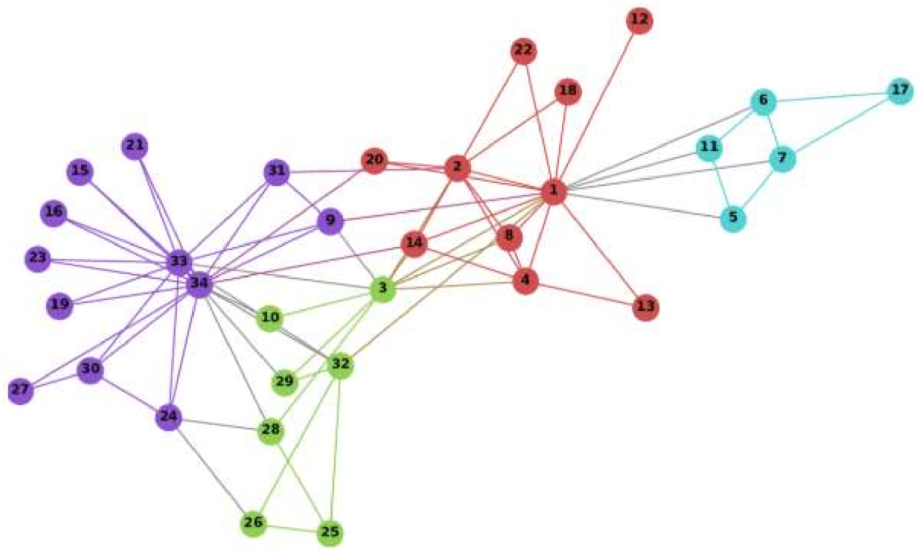
- Vertices (Nodes) V
- Edges (Connections) E (Directed or Undirected)

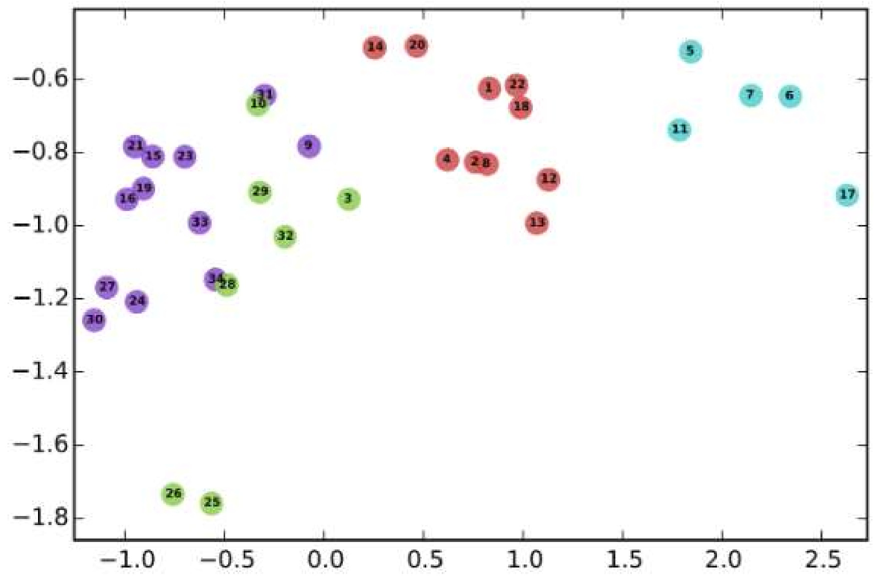
Words and images are a special case of graphs



Introduction. Graphs Representation

Most of the time: node representation

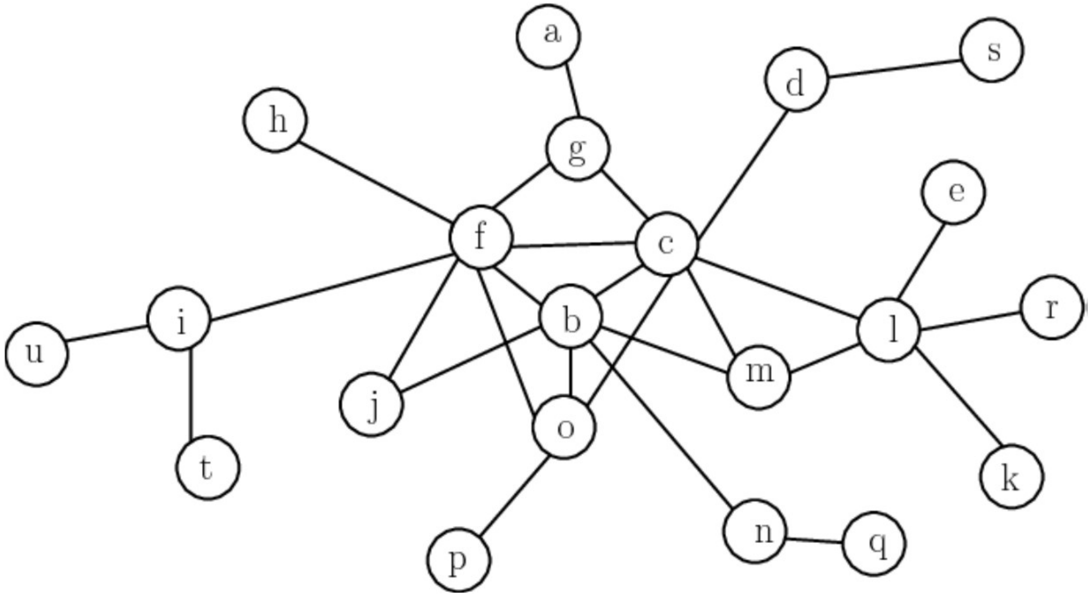




Source: Google AI blog
Left: The well-known [Karate](#) graph representing a social network.
Right: A continuous space embedding of the nodes in the graph using [DeepWalk](#).

Introduction. Graphs Representation

The problem is graphs are not linear.
If we could sample multiple random linear sequence from graphs, then we could pass them to word2vec algorithm (etc. skip-gram).

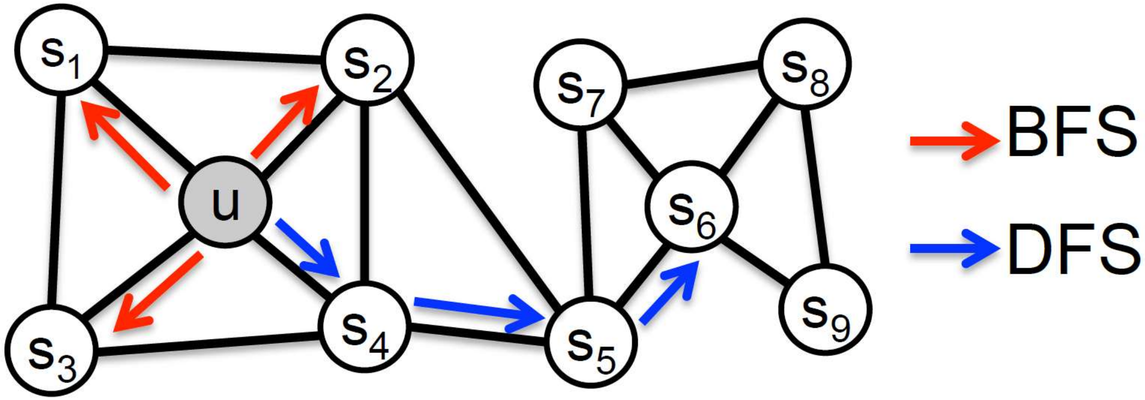


Introduction. BFS & DFS

Suppose *k* is the size neighborhood = 3

BFS samples: $s_1\ s_2\ s_3$

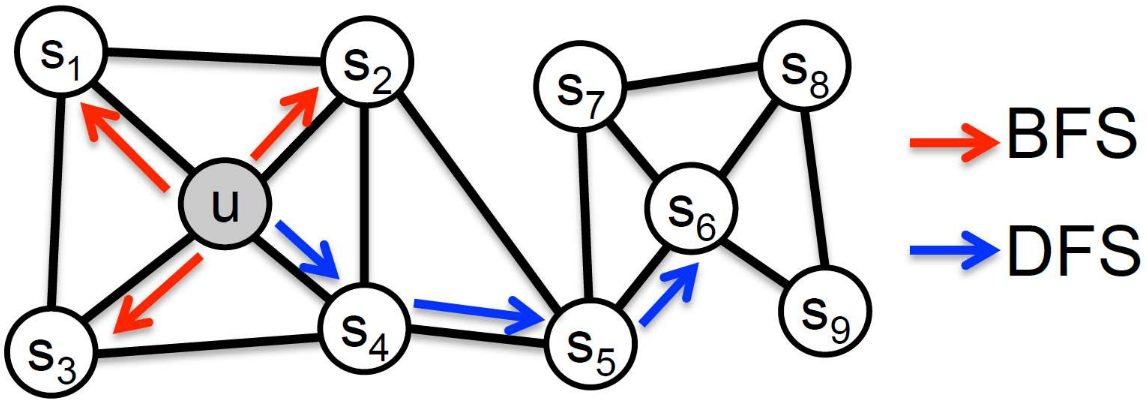
DFS samples: $s_4\ s_5\ s_6$



BFS and DFS search strategies from node u (k = 3)
Source: node2vec: Scalable Feature Learning for Networks

Introduction. Homophily & Structural Equivalence

Homophily: similar network clusters (ex: s_1 and u)
Structural equivalence: similar structural roles (ex: s_6 and u)
BFS closely lead to structural embeddings
DFS closely lead to homophily



BFS and DFS search strategies from node u (k = 3)
Source: node2vec: Scalable Feature Learning for Networks

Introduction. Problem statement

PROBLEMS

- Unsupervised feature learning (e.g., PCA) suffer from computational costs because eigen decomposition is expensive
- If we turn a network into a ordered sequence of nodes, we can pass it to word2vec
- There are many possible sampling strategies
- The MAJOR GAP is that there is no flexibility in sampling nodes from a network

Introduction. Key Contribution

OBJECTIVE

To design **a flexible sampling technique that is not tied to a particular sampling strategy and provides hyper-parameters to tune the explored search space.**

Methodology - Feature learning framework

Let G = (V;E)

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

Every $u \in V$, $N_s(u) \subset V$ as a network neighborhood

Skip-gram architecture

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

Networks are not linear, and thus richer notion of a neighborhood is needed

$N_s(u)$ -> vastly different structures depending on the sampling strategy S

Methodology - Biased random walk

2nd order random walk with two hyper-parameters p and q
2nd order means that it considers the previous state where it came from

Unnormalized transition probability:

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

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

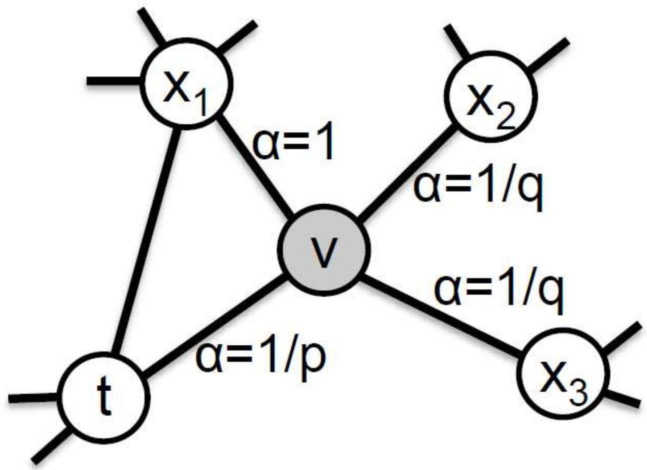


Illustration of the random walk procedure in node2vec. The walk just transitioned from t to v and is now evaluating its next step out of node v. Edge labels indicate search biases
Source: node2vec: Scalable Feature Learning for Networks

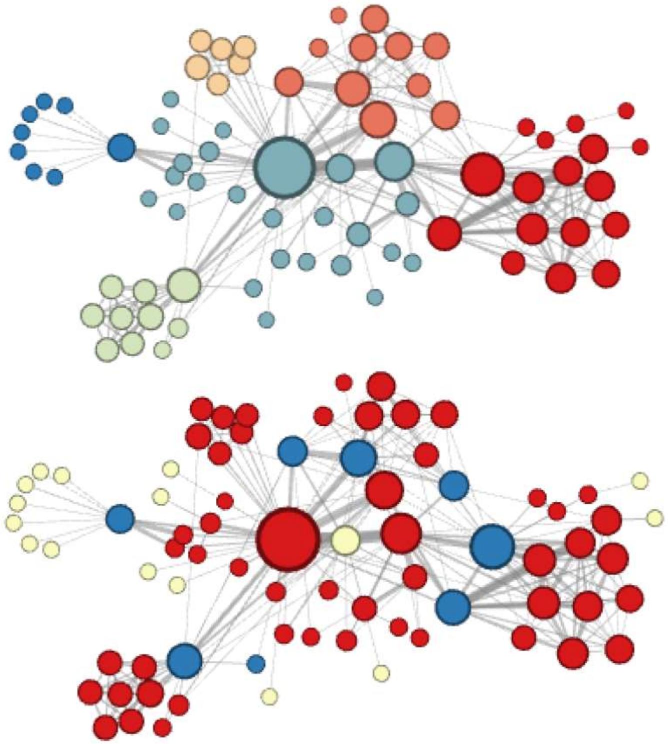
Methodology - The node2vec algorithm

Algorithm 1 The *node2vec* algorithm.

LearnFeatures (Graph $G = (V, E, W)$, Dimensions d, Walks per node r, Walk length l, Context size k, Return p, In-out q)
  π = PreprocessModifiedWeights(G, p, q)
  $G' = (V, E, \pi)$
  Initialize $walks$ to Empty
  for $iter = 1$ **to** r **do**
    for all nodes $u \in V$ **do**
      $walk$ = node2vecWalk(G', u, l)
      Append $walk$ to $walks$
  f = StochasticGradientDescent$(k, d, walks)$
  return f

node2vecWalk (Graph $G' = (V, E, \pi)$, Start node u, Length l)
  Inititalize $walk$ to $[u]$
  for $walk\_iter = 1$ **to** l **do**
    $curr = walk[-1]$
    V_{curr} = GetNeighbors$(curr, G')$
    s = AliasSample(V_{curr}, π)
    Append s to $walk$
  return $walk$

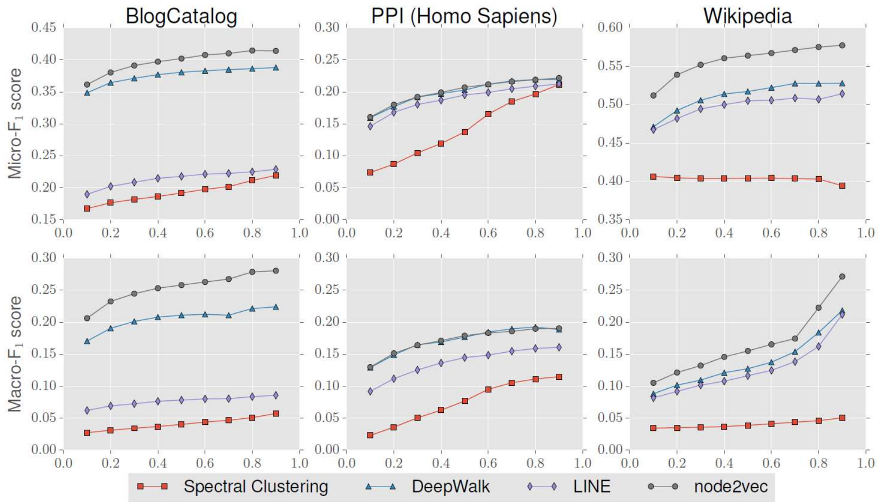
Results and Discussions



Complementary visualizations of Les Misérables coappearance network generated by node2vec with label colours reflecting homophily (top) and structural equivalence (bottom).
Source: node2vec: Scalable Feature Learning for Networks

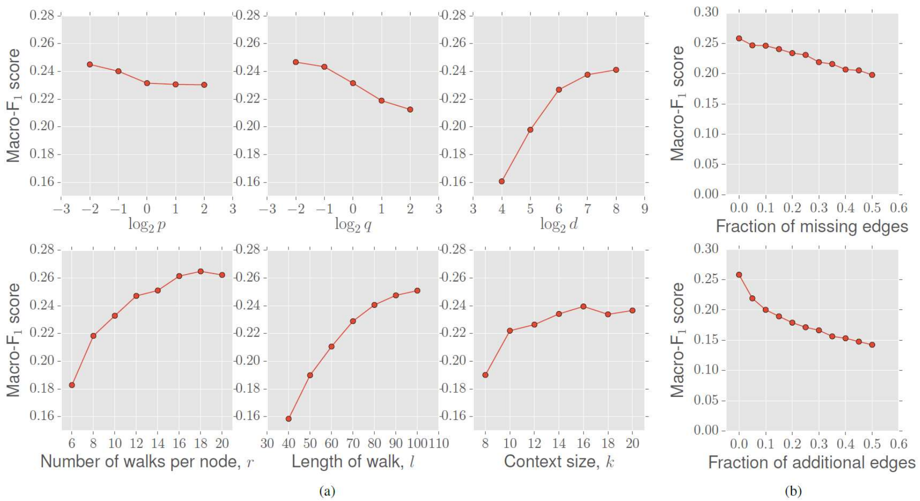
Algorithm	**Dataset**		
	BlogCatalog	PPI	Wikipedia
Spectral Clustering	0.0405	0.0681	0.0395
DeepWalk	0.2110	0.1768	0.1274
LINE	0.0784	0.1447	0.1164
node2vec	**0.2581**	**0.1791**	**0.1552**
node2vec settings (p,q)	0.25, 0.25	4, 1	4, 0.5
Gain of *node2vec* [%]	**22.3**	**1.3**	**21.8**

Macro-F1 scores for multilabel classification on BlogCatalog, PPI (Homo sapiens) and Wikipedia word cooccurrence networks with 50% of the nodes labelled for training.

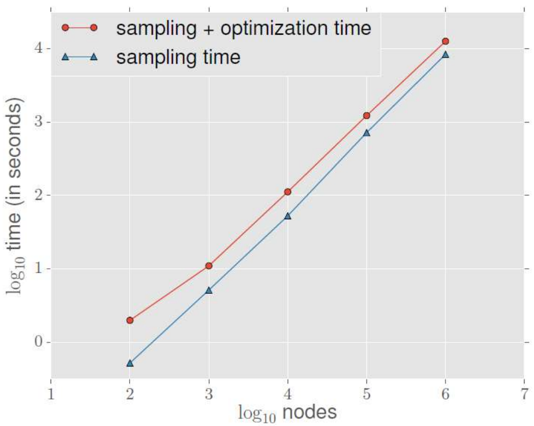


Performance evaluation of different benchmarks on varying the amount of labelled data used for training. The x axis denotes the fraction of labelled data

Results and Discussions



(a). Parameter sensitivity (b). Perturbation analysis for multilabel classification on the BlogCatalog network.



Scalability of node2vec on Erdos-Renyi graphs with an average degree of 10.

Op	**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
(a)	Spectral Clustering	0.5960	0.6588	0.5812
	DeepWalk	0.7238	0.6923	0.7066
	LINE	0.7029	0.6330	0.6516
	node2vec	0.7266	0.7543	0.7221
(b)	Spectral Clustering	0.6192	0.4920	0.5740
	DeepWalk	**0.9680**	0.7441	0.9340
	LINE	0.9490	0.7249	0.8902
	node2vec	**0.9680**	**0.7719**	**0.9366**
(c)	Spectral Clustering	0.7200	0.6356	0.7099
	DeepWalk	0.9574	0.6026	0.8282
	LINE	0.9483	0.7024	0.8809
	node2vec	0.9602	0.6292	0.8468
(d)	Spectral Clustering	0.7107	0.6026	0.6765
	DeepWalk	0.9584	0.6118	0.8305
	LINE	0.9460	0.7106	0.8862
	node2vec	0.9606	0.6236	0.8477

Area Under Curve (AUC) scores for link prediction. Comparison with popular baselines and embedding based methods bootstapped using binary operators: (a) Average, (b) Hadamard, (c) Weighted-L1, and (d) Weighted-L2

Conclusions

- BFS suitable for structural equivalences
- DFS suitable for homophiles clusters
- node2vec is both flexible and controllable exploring neighborhoods through parameters p and q