The journey from Math to ML

“node2vec: Scalable Feature Learning for Networks”
Episode 9

node2vec: Scalable feature learning for networks

A Grover, J Leskovec - Proceedings of the 22nd ACM SIGKDD …, 2016 - dl.acm.org

Prediction tasks over nodes and edges in networks require careful effort in engineering features used by learning algorithms. Recent research in the broader field of representation learning has led to significant progress in automating prediction by learning the features themselves. However, present feature learning approaches are not expressive enough to capture the diversity of connectivity patterns observed in networks. Here we propose node2vec, an algorithmic framework for learning continuous feature representations for …

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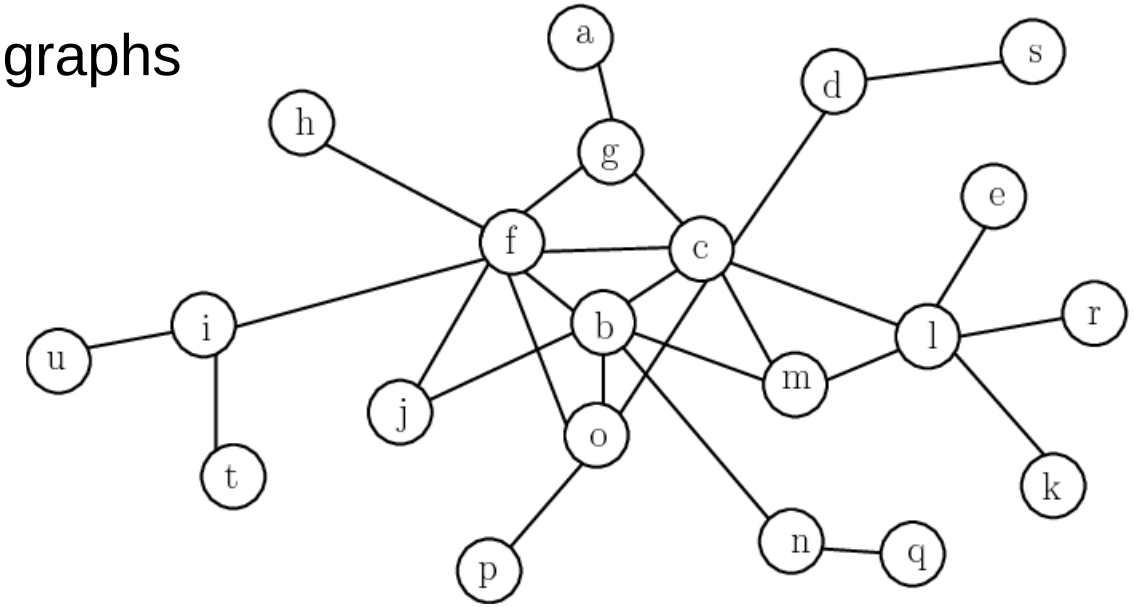
Contents

Introduction. Graphs

Data consist of

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

Words and images are a special case of graphs

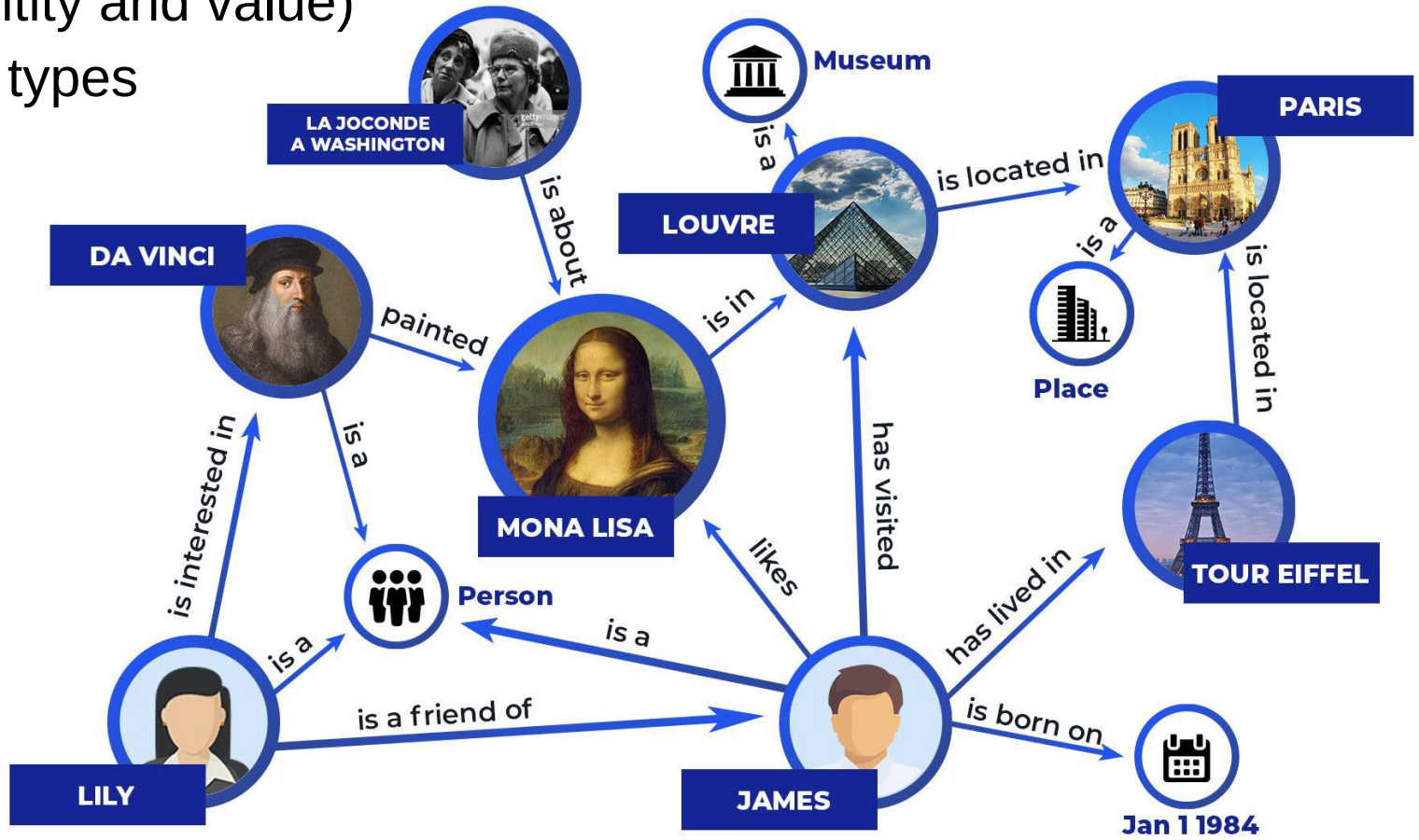


Introduction. Graphs

Everything is a graph

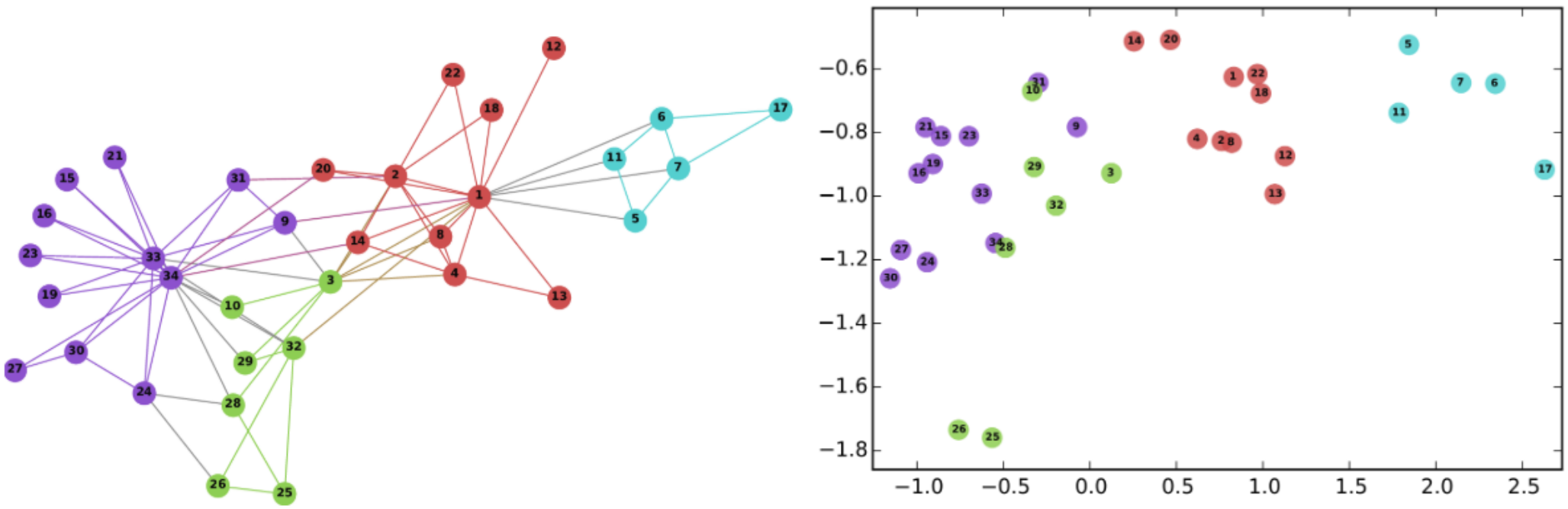
Example:

- Multiple node types (entity and value)
- Directed Multiple edge types



Introduction. Graphs Representation

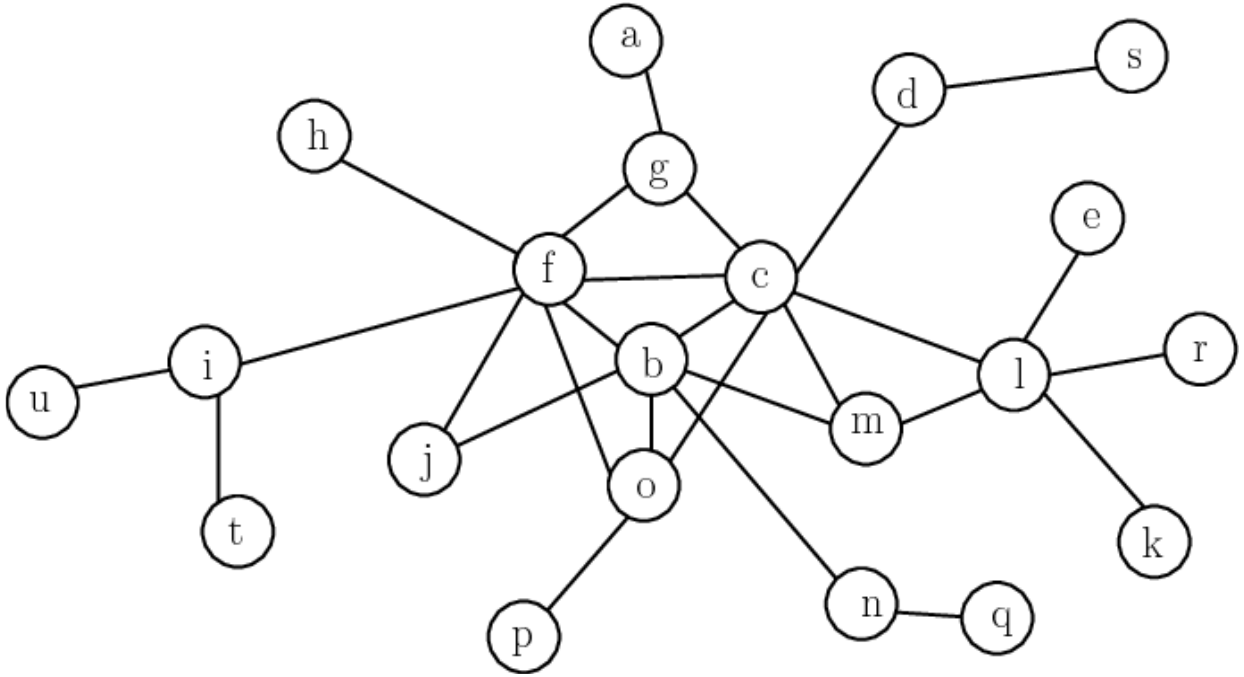
Most of the time: node representation



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. Homophily & Structural Equivalence

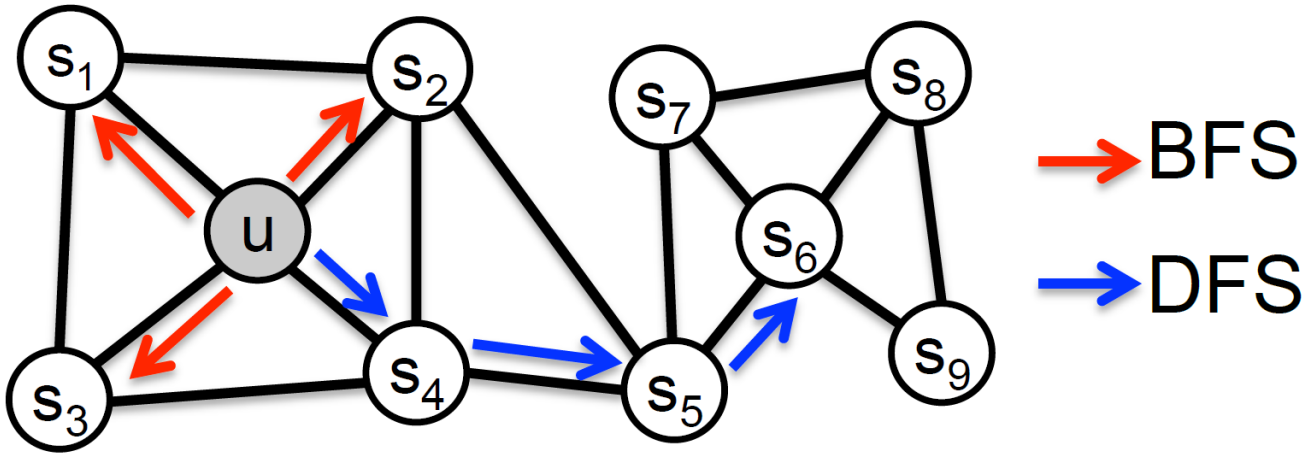
What kind of representation do we want?

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



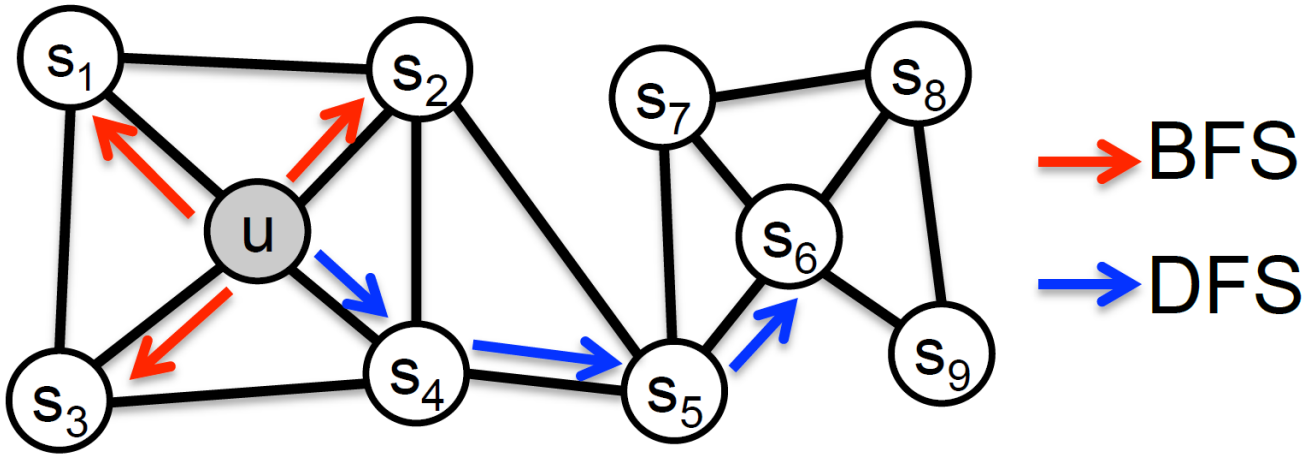
BFS and DFS search strategies from node u (k = 3)
Source: node2vec: Scalable Feature Learning for Networks

Introduction. BFS & DFS

Suppose *k* is the size of 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. 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 of node u generated through a neighborhood sampling strategy S

Extending the Skip-gram architecture to networks

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

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

The neighborhoods are not restricted just immediate neighbors but can have vastly different structures depending on the sampling strategy S

Simply, how do we decide which nodes are neighbors given u

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:

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

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

Normalized transition probability:

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

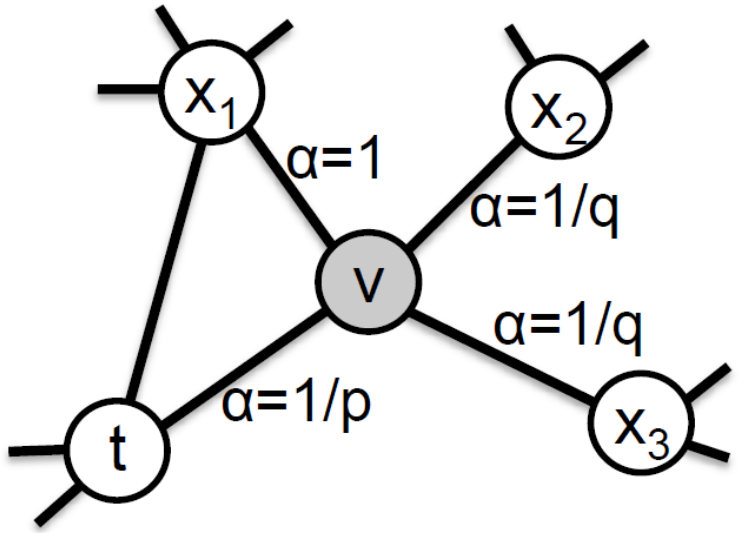


Illustration of the random walk procedure in node2vec. The walk just transitioned from t to v and is now evaluating its next step out of node v. Edge labels indicate search biases
Source: node2vec: Scalable Feature Learning for Networks

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 $walk$

Methodology - Learning edge features

Given two nodes u and v

We can define $g(u, v) = f(u) \circ f(v)$

Such that $g: V \times V \rightarrow \mathbb{R}^d$

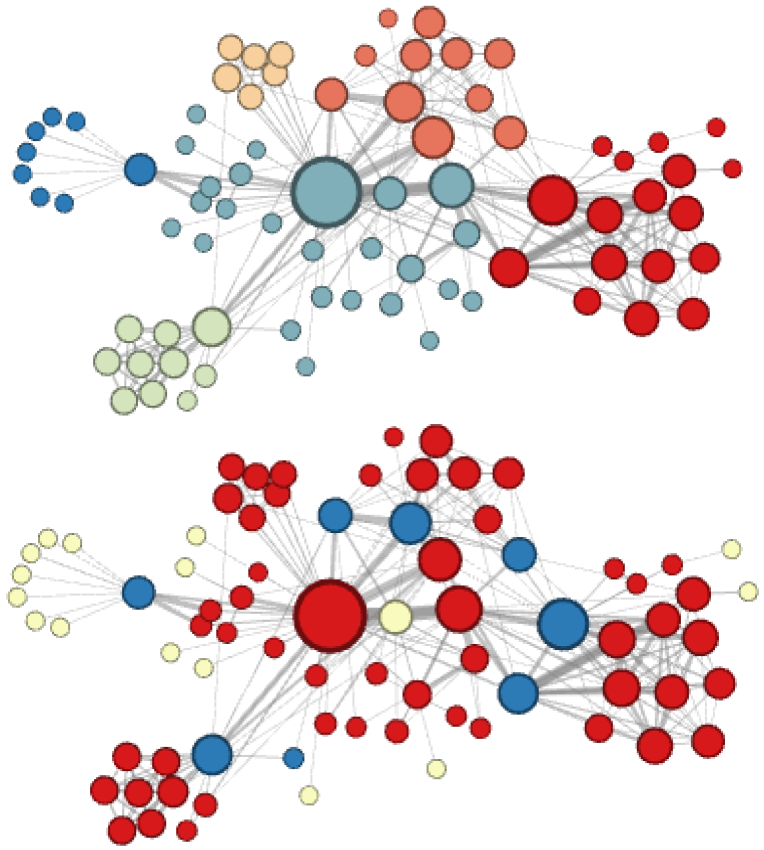
Choice of binary operators $\circ$ could be

- Average
- Hadamard
- L1 norm
- L2 norm
- …

For example, we could predict whether a link exist between two nodes

Binary classification task

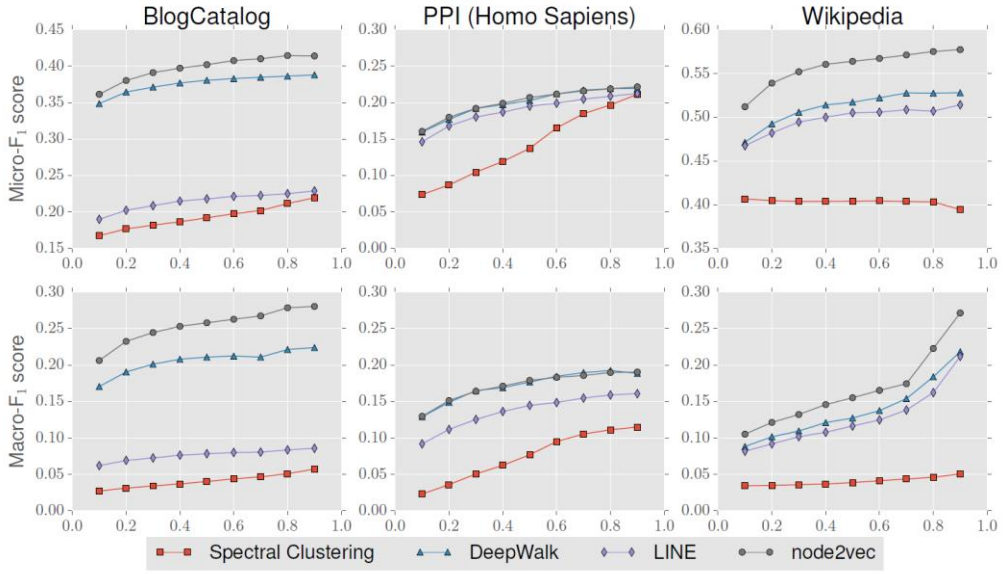
Results and Discussions



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

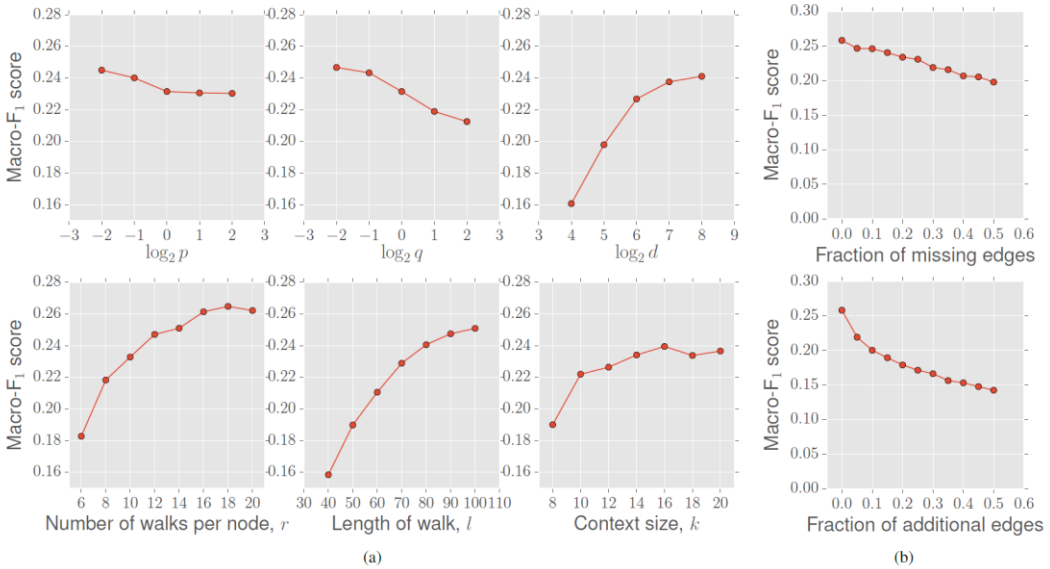
Algorithm	Dataset		
	BlogCatalog	PPI	Wikipedia
Spectral Clustering	0.0405	0.0681	0.0395
DeepWalk	0.2110	0.1768	0.1274
LINE	0.0784	0.1447	0.1164
node2vec	**0.2581**	**0.1791**	**0.1552**
node2vec settings (p,q)	0.25, 0.25	4, 1	4, 0.5
Gain of *node2vec* [%]	**22.3**	**1.3**	**21.8**

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

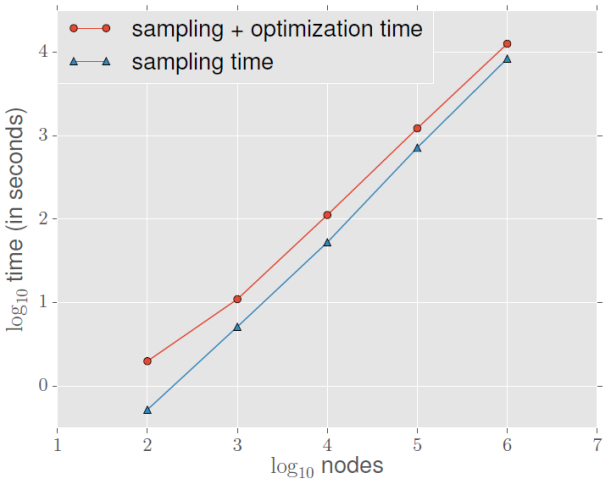


Performance evaluation of different benchmarks on varying the amount of labelled data used for training. The x axis denotes the fraction of labelled data

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 bootstrapped 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
- node2vec is scalable and robust to perturbations

Future work:

- To explore the reason why Hadamard operator is success in the link prediction task