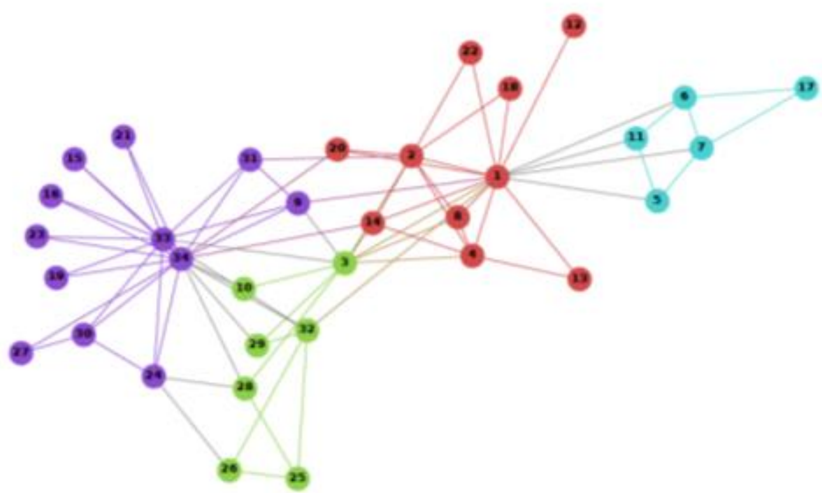
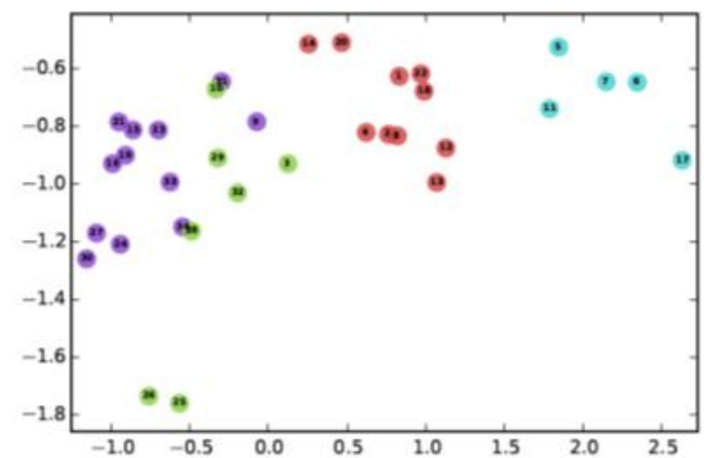
CISC 372 Network/Graph Embedding



Input



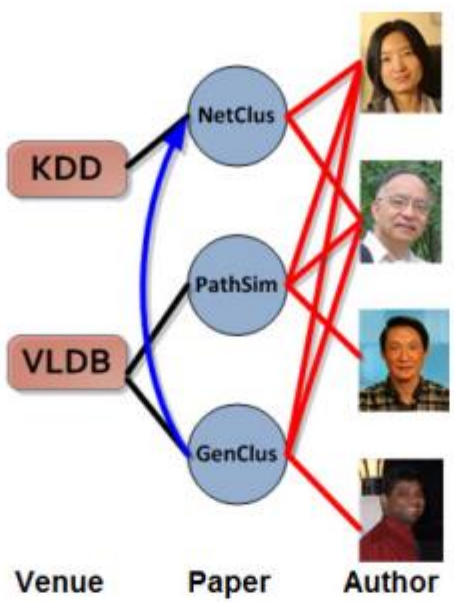
Output

Graph Embedding — Representation Learning on Networks, snap.stanford.edu/proj/embeddings-www

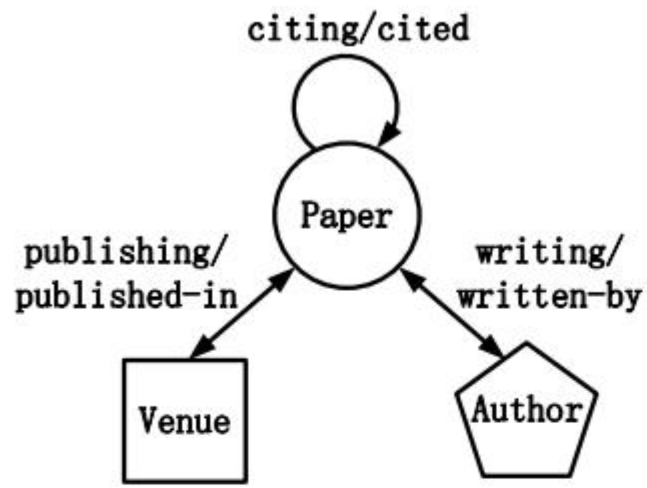
- Part III: Network
  - Basic characteristics of network
  - Recommendation
  - ***Supervised/Self-supervised learning on information network***
  - PageRank

Graph Types

- Homogeneous Network vs Heterogenous Information Network

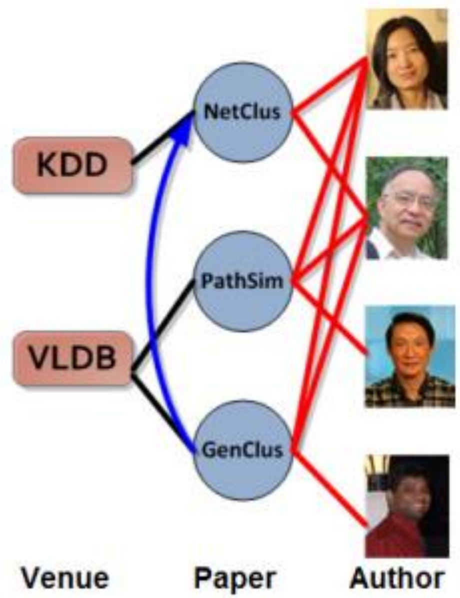


(a) Network instance

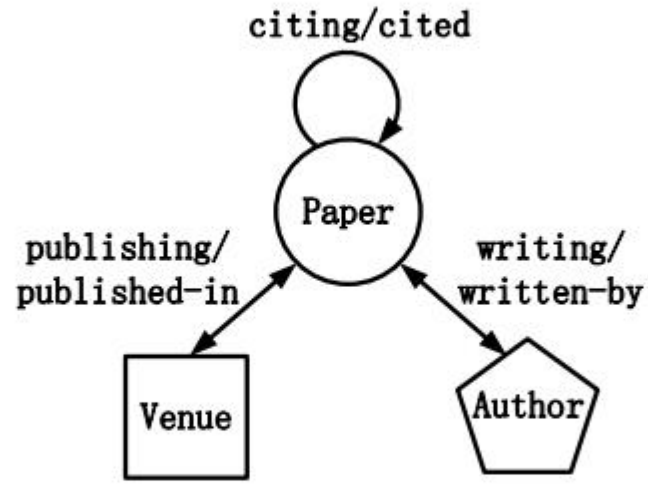


(b) Network schema

Graph Types



(a) Network instance

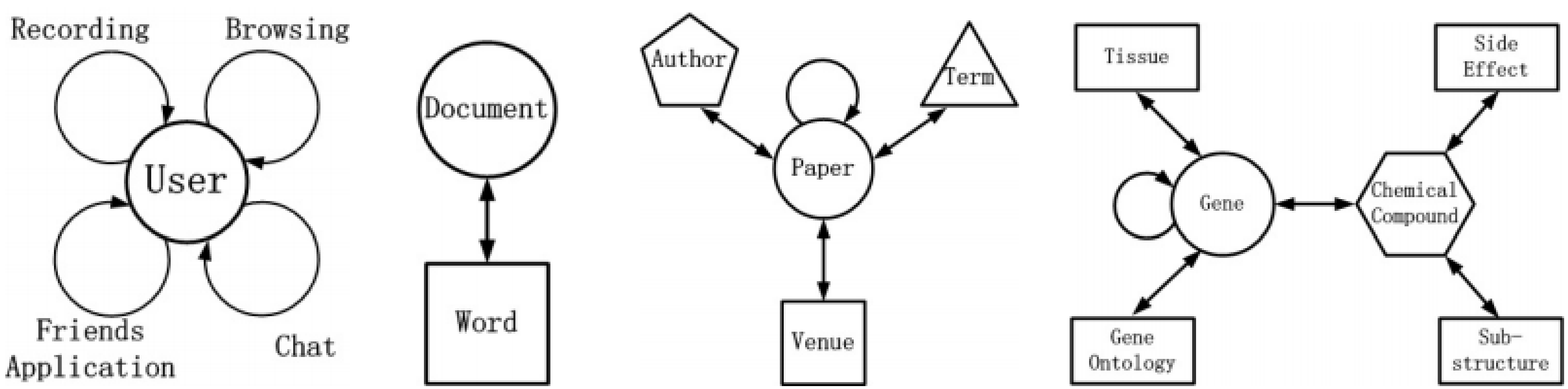


(b) Network schema

DEFINITION 2: **Heterogeneous/homogeneous information Network**. The information network is called **heterogeneous information network** if the types of objects $|\mathcal{A}| > 1$ or the types of relations $|\mathcal{R}| > 1$; otherwise, it is a **homogeneous information network**.

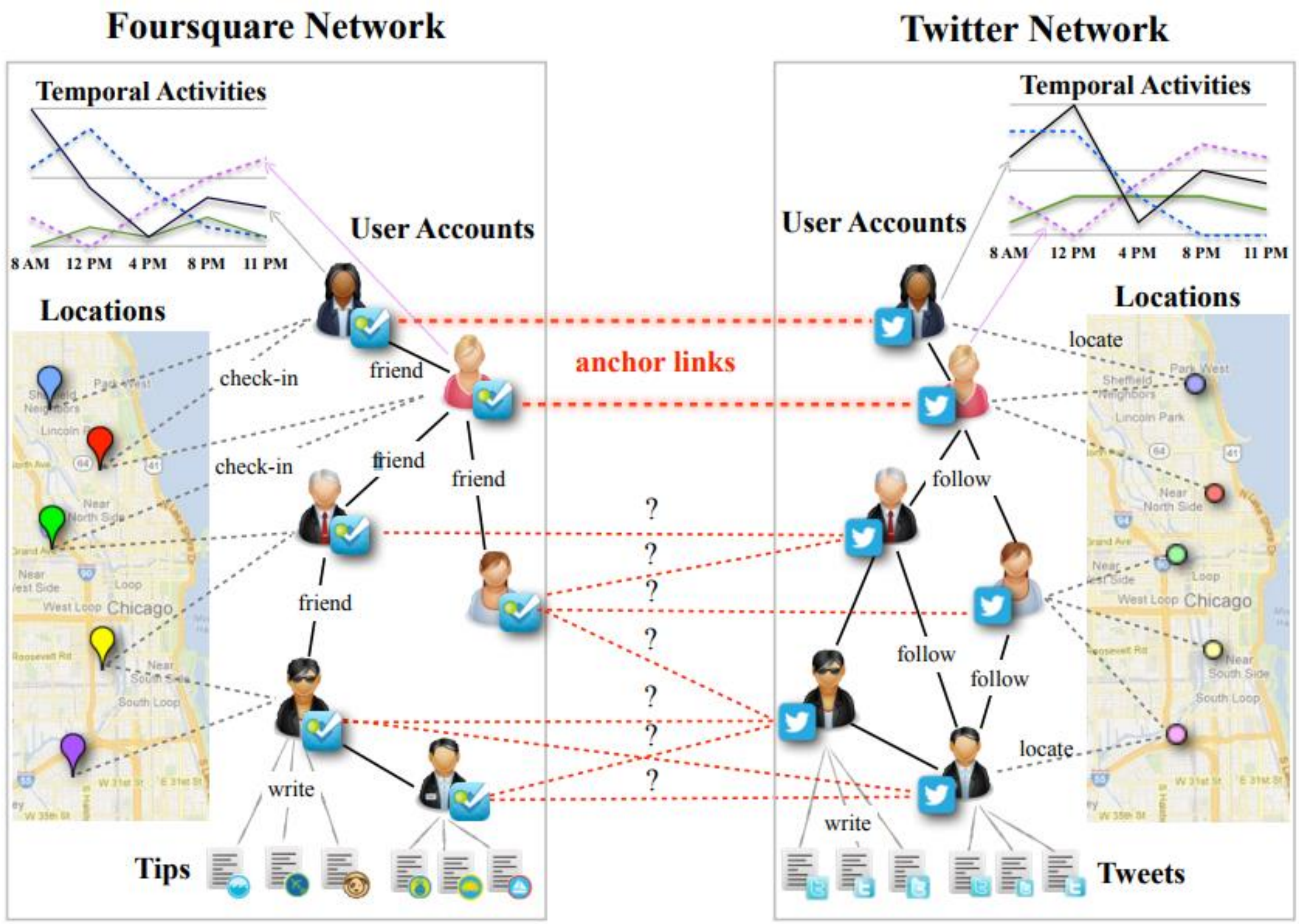
Graph Types

- Heterogenous Information Network
  - Example graph?
  - Social Media Platform
    - Users, Tags, Posts
  - Health Care System:
    - Doctors, Patients, Diseases, Devices



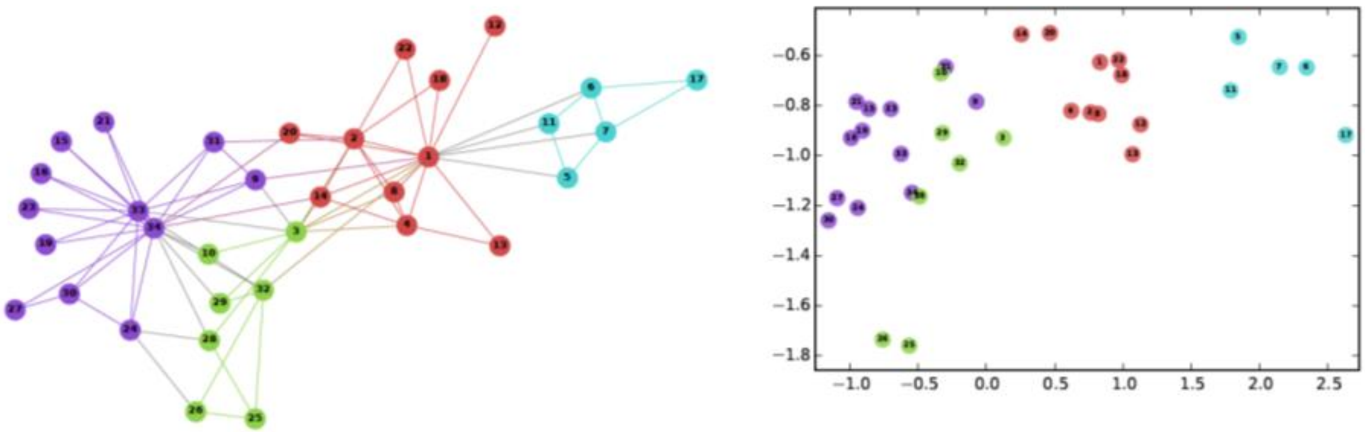
(a) Multi-relation (b) Bipartite (c) Star-schema (d) Multiple-hub

Reality is much more complicated



Assumption

- Graph Data
  - lie in a low dimensional manifold

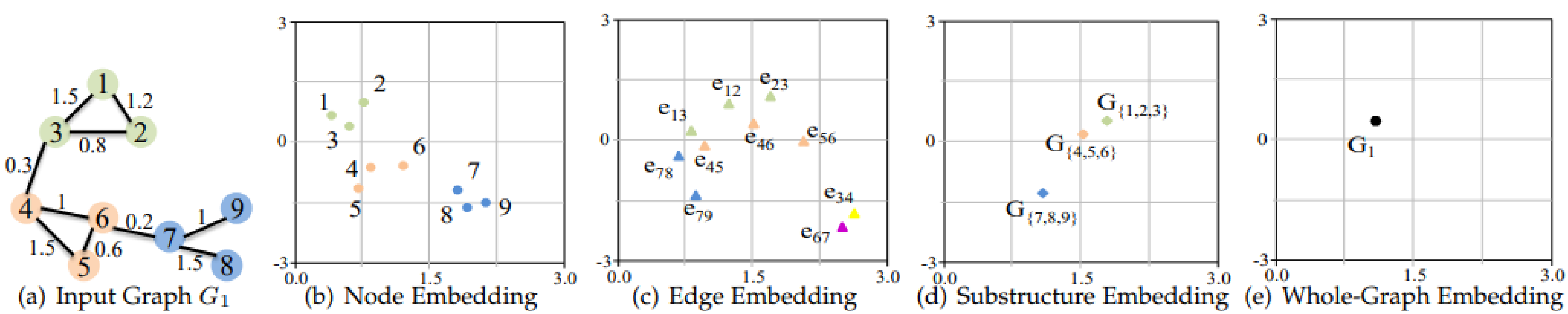


Input Output

- Complex non-relational graph structure -> low dimensional embedding space

Why Graph Embedding

- Latent Embedding -> Hidden Regularities of the Data
- Similar to Language Model, useful for a lot of downstream task
  - Link prediction
  - Node prediction
  - Recommendation
  - Tag Prediction



Graph Embedding Problem Settings

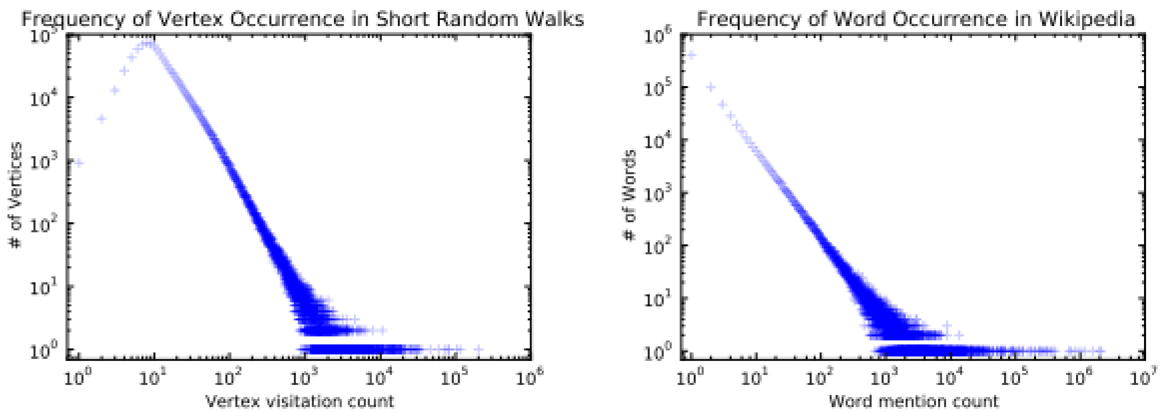
- Graph Embedding Input
  - Homogeneous Graph
  - Heterogeneous Graph
  - Graph with Auxiliary Information
  - Graph Constructed from Non-relational Data
- Graph Embedding Output
  - Node Embedding
  - Edge Embedding
  - Hybrid Embedding
  - Whole-Graph Embedding

Graph Embedding Techniques

- Matrix Factorization
  - Graph Laplacian Eigenmaps
  - Node Proximity Matrix Factorization
- Deep Learning
  - With Random Walk
  - Without Random Walk
- Edge Reconstruction
  - Maximize Edge Reconstruct Probability
  - Minimize Distance-based Loss
  - Minimize Margin-based Ranking Loss
- Graph Kernel
  - Based on Graphlet
  - Based on Subtree Patterns
  - Based on Random Walks
- Generative Model
  - Embed Graph into Latent Space
  - Incorporate Semantics for Embedding

DeepWalk

- Basic Idea -> Graph is similar to Text!
  - (if we randomly travel to through the graph)
  - Connection: Power laws



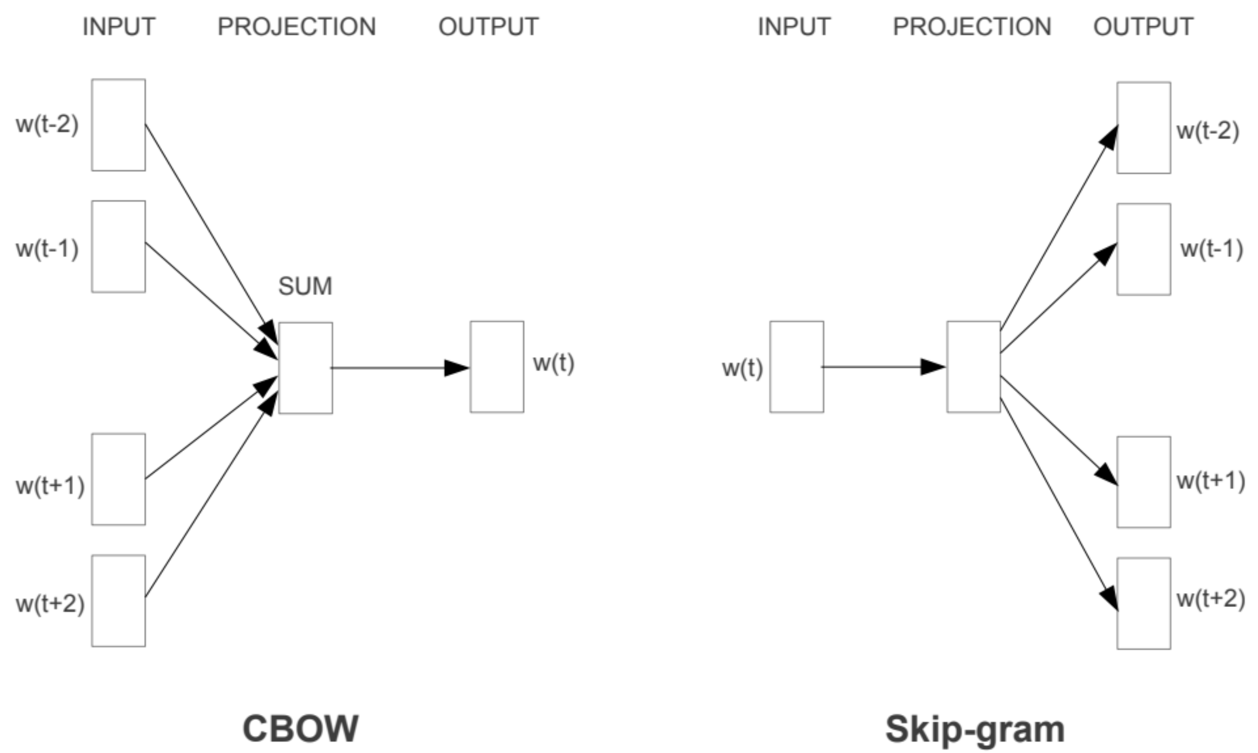
(a) YouTube Social Graph (b) Wikipedia Article Text

Figure 2: The power-law distribution of vertices appearing in short random walks (2a) follows a power-law, much like the distribution of words in natural language (2b).

Perozzi, B., Al-Rfou, R., & Skiena, S. (2014, August). Deepwalk: Online learning of social representations. In *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining* (pp. 701-710).

DeepWalk

- Word2Vec
  - Recall:



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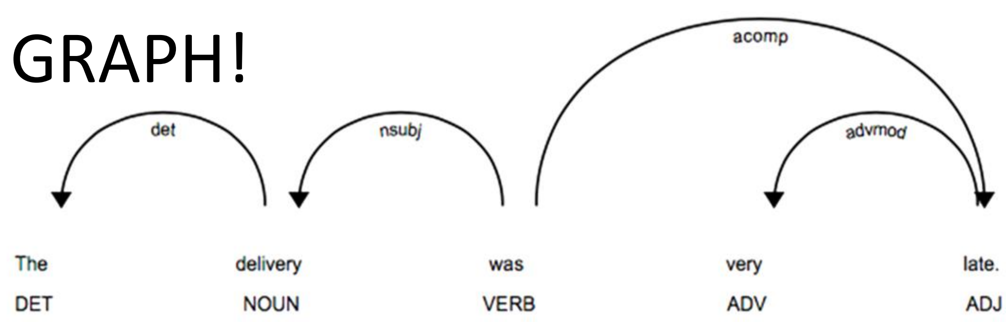
DeepWalk

- Word2Vec
  - Create questions (and true answers) from the dataset to train the model.
  - The, baby, is, **smiling**, at, her, mom
    - Question: The, baby, is, ___, at, her, mom
    - Answer: smiling
  - The, baby, is, **flying**, at, her, mom
    - Question: The, baby, is, ___, at, her, mom
    - Answer: flying
- In fact, Sentence is GRAPH!



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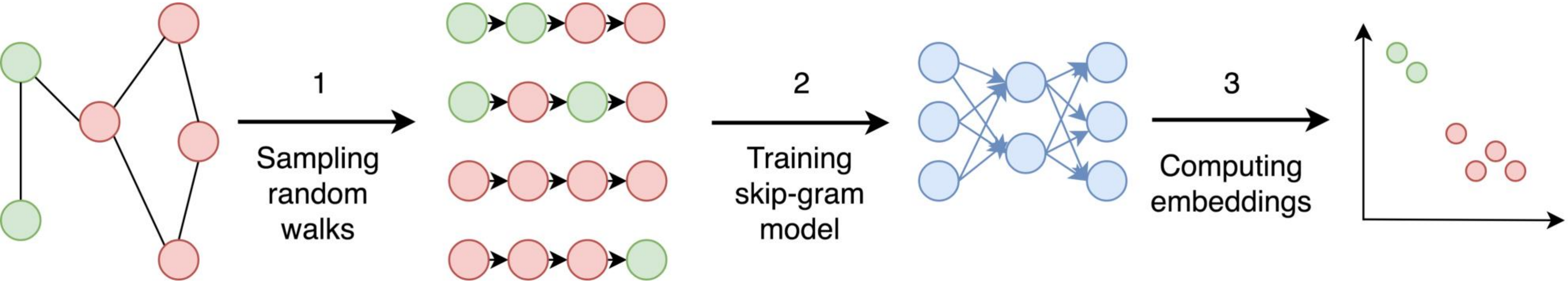
DeepWalk



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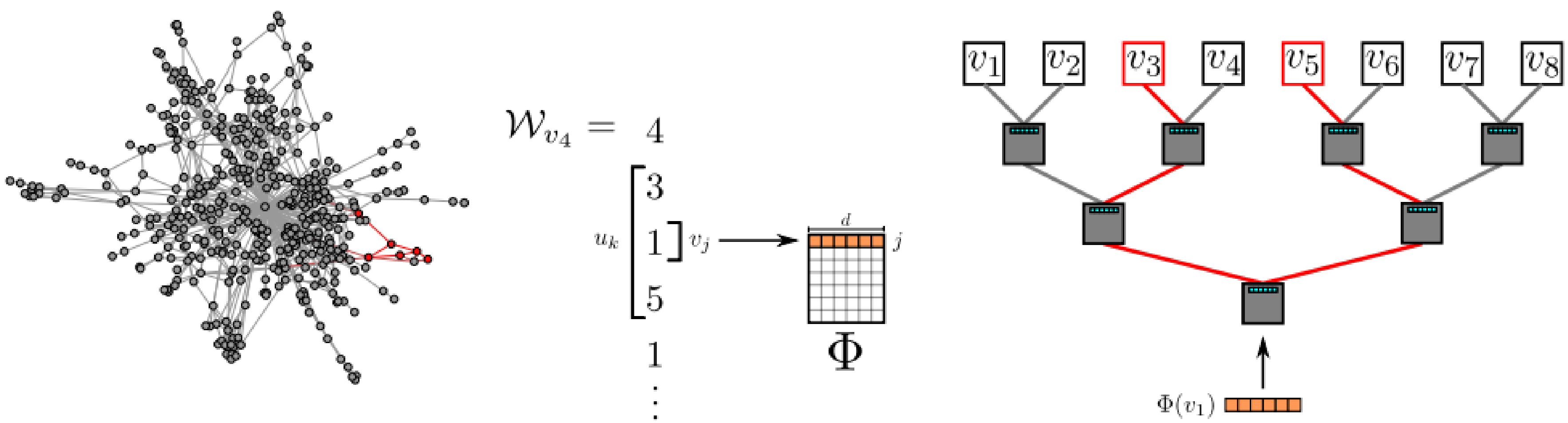
DeepWalk

- Three steps:
  - Sequence Generation (random walk)
  - Representation mapping (embedding layer)
  - Prediction (through word2vec)



(a) Random walk generation. (b) Representation mapping. (c) Hierarchical Softmax.

Perozzi, B., Al-Rfou, R., & Skiena, S. (2014, August). Deepwalk: Online learning of social representations. In *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining* (pp. 701-710).

DeepWalk

- Performance?
  - BlogCataLog classification
  - Flicker label prediction
  - Youtube Label Prediction

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DeepWalk

	% Labeled Nodes	10%	20%	30%	40%	50%	60%	70%	80%	90%
Micro-F1(%)	DeepWalk	**36.00**	**38.20**	**39.60**	**40.30**	**41.00**	**41.30**	41.50	41.50	42.00
	SpectralClustering	31.06	34.95	37.27	38.93	39.97	40.99	**41.66**	**42.42**	**42.62**
	EdgeCluster	27.94	30.76	31.85	32.99	34.12	35.00	34.63	35.99	36.29
	Modularity	27.35	30.74	31.77	32.97	34.09	36.13	36.08	37.23	38.18
	wvRN	19.51	24.34	25.62	28.82	30.37	31.81	32.19	33.33	34.28
	Majority	16.51	16.66	16.61	16.70	16.91	16.99	16.92	16.49	17.26
Macro-F1(%)	DeepWalk	**21.30**	**23.80**	25.30	26.30	27.30	27.60	27.90	28.20	28.90
	SpectralClustering	19.14	23.57	**25.97**	**27.46**	**28.31**	**29.46**	**30.13**	**31.38**	**31.78**
	EdgeCluster	16.16	19.16	20.48	22.00	23.00	23.64	23.82	24.61	24.92
	Modularity	17.36	20.00	20.80	21.85	22.65	23.41	23.89	24.20	24.97
	wvRN	6.25	10.13	11.64	14.24	15.86	17.18	17.98	18.86	19.57
	Majority	2.52	2.55	2.52	2.58	2.58	2.63	2.61	2.48	2.62

Table 2: Multi-label classification results in BlogCatalog

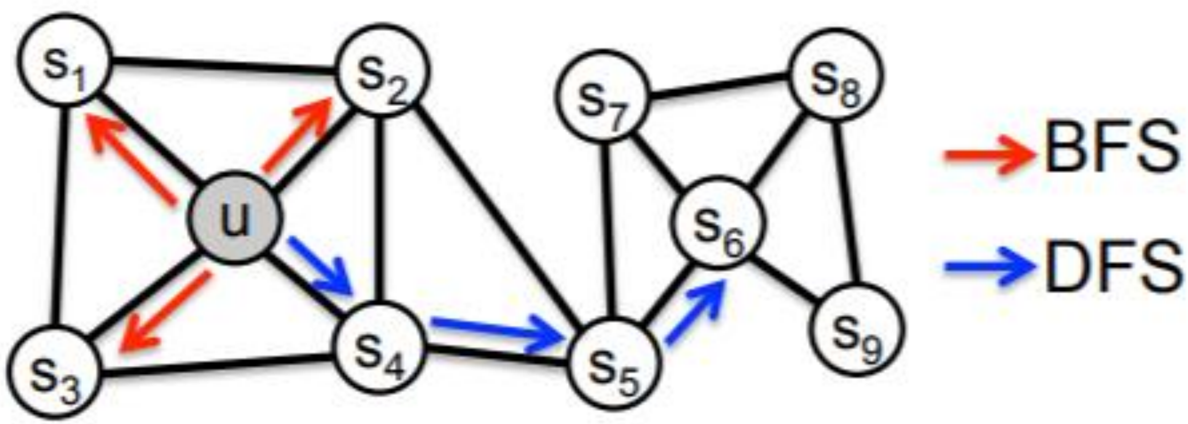
	% Labeled Nodes	1%	2%	3%	4%	5%	6%	7%	8%	9%	10%
Micro-F1(%)	DeepWalk	**32.4**	**34.6**	**35.9**	**36.7**	**37.2**	**37.7**	**38.1**	**38.3**	**38.5**	**38.7**
	SpectralClustering	27.43	30.11	31.63	32.69	33.31	33.95	34.46	34.81	35.14	35.41
	EdgeCluster	25.75	28.53	29.14	30.31	30.85	31.53	31.75	31.76	32.19	32.84
	Modularity	22.75	25.29	27.3	27.6	28.05	29.33	29.43	28.89	29.17	29.2
	wvRN	17.7	14.43	15.72	20.97	19.83	19.42	19.22	21.25	22.51	22.73
	Majority	16.34	16.31	16.34	16.46	16.65	16.44	16.38	16.62	16.67	16.71
Macro-F1(%)	DeepWalk	**14.0**	17.3	**19.6**	**21.1**	**22.1**	**22.9**	**23.6**	**24.1**	**24.6**	**25.0**
	SpectralClustering	13.84	**17.49**	19.44	20.75	21.60	22.36	23.01	23.36	23.82	24.05
	EdgeCluster	10.52	14.10	15.91	16.72	18.01	18.54	19.54	20.18	20.78	20.85
	Modularity	10.21	13.37	15.24	15.11	16.14	16.64	17.02	17.1	17.14	17.12
	wvRN	1.53	2.46	2.91	3.47	4.95	5.56	5.82	6.59	8.00	7.26
	Majority	0.45	0.44	0.45	0.46	0.47	0.44	0.45	0.47	0.47	0.47

Table 3: Multi-label classification results in Flickr

Perozzi, B., Al-Rfou, R., & Skiena, S. (2014, August). Deepwalk: Online learning of social representations. In *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining* (pp. 701-710).

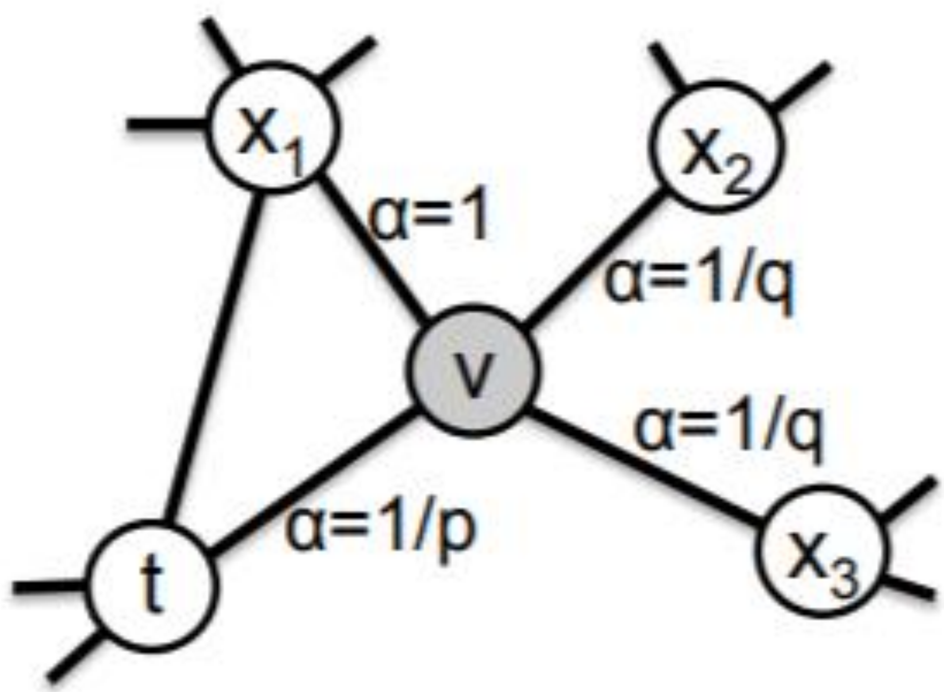
Node2Vec

- Second order traversal
  - Breadth-first Sampling (BFS)
  - Depth-first Sampling (DFS)
  - BFS, DFS traversal yields very different sequence
  - BFS -> emphasize 1st order neighbor
  - DFS -> emphasize >2nd order neighbor



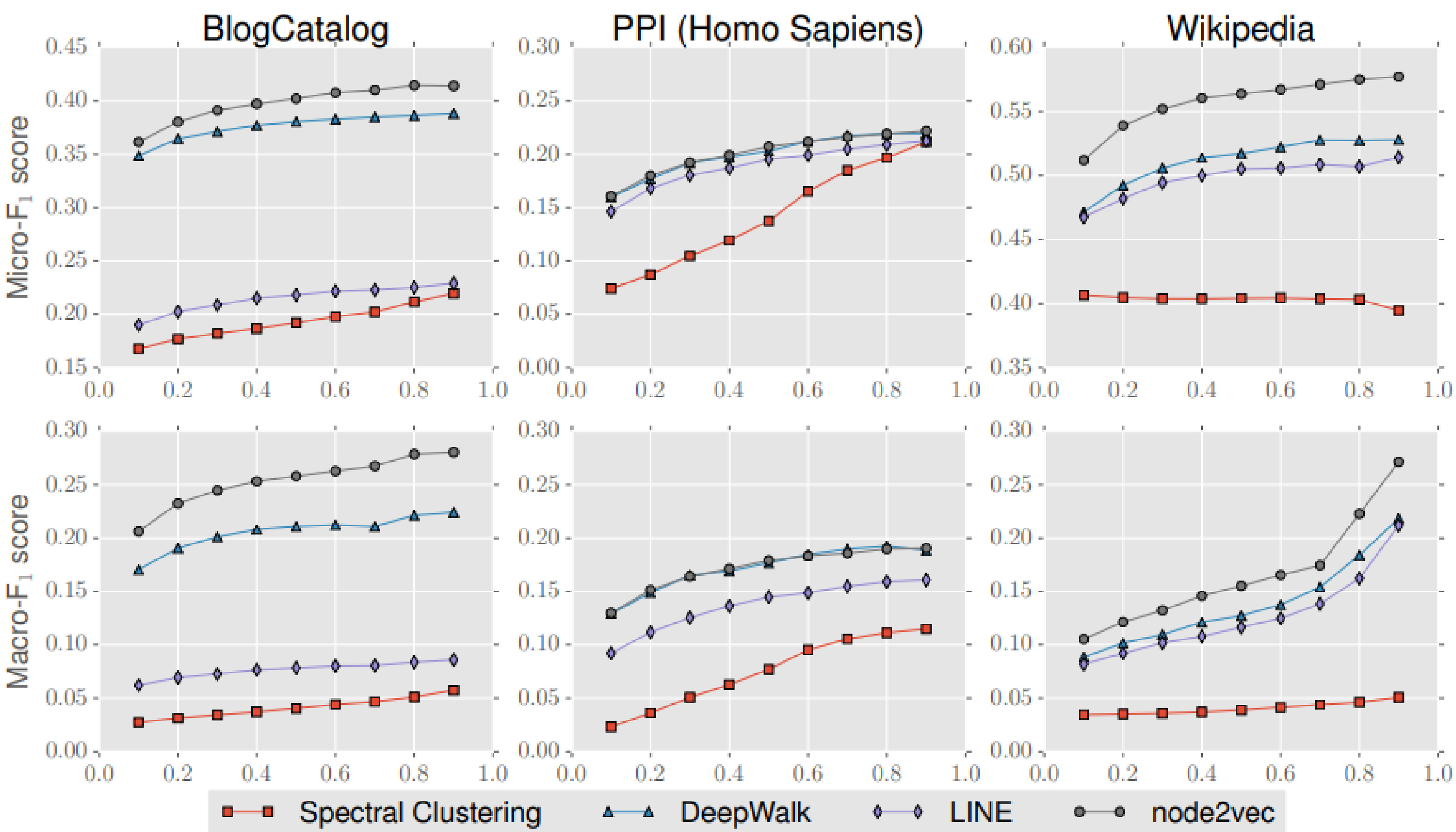
Node2Vec

- Controlled Random Walk
  - p — return rate
    q — exploration rate



Node2Vec

- Learning? Same as DeepWalk and Word2Vec



LINE

- Edge sampling instead of random walk
- Separate embedding space into
  - 1^{st} order proximity
  - 2^{nd} order proximity
- Avoid sequence generation
- More efficient and scalable
- the consideration of the second order proximity effectively complements the sparsity of the first-order proximity and better preserves the global structure of the network.

LINE

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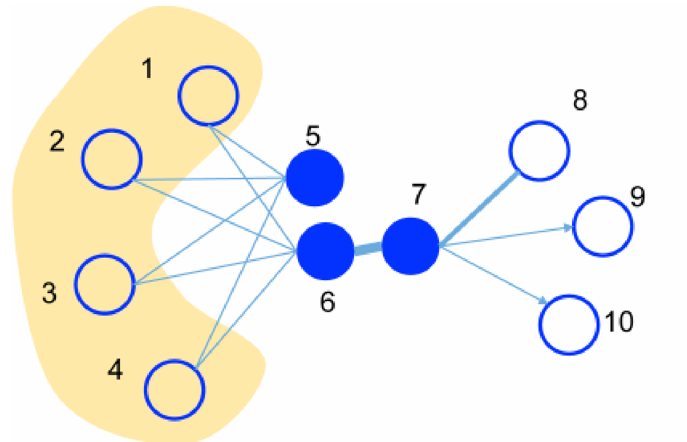

- Avoid sequence generation
- More efficient and scalable
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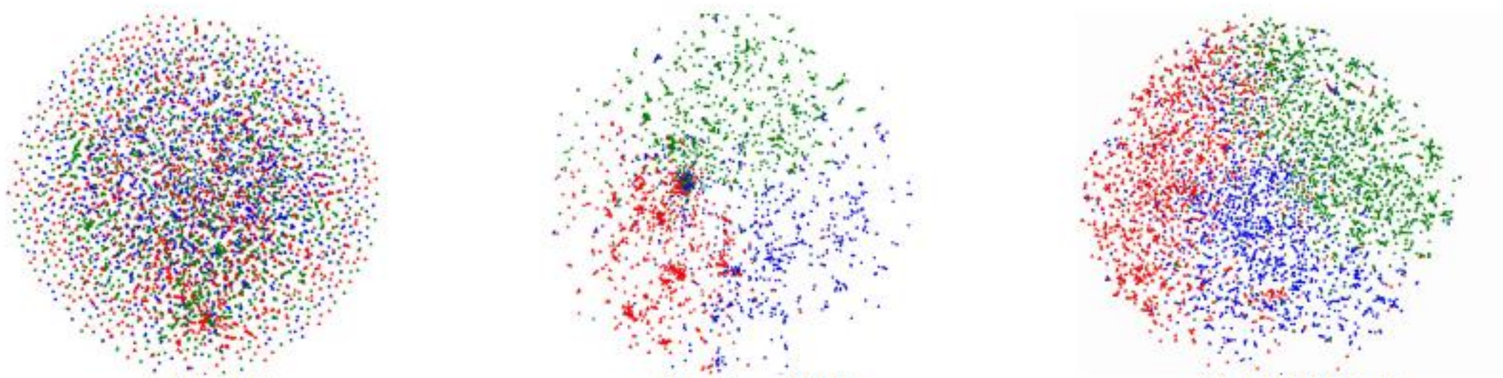
LINE

Table 3: Results of Wikipedia page classification on WIKIPEDIA data set.

Metric	Algorithm	10%	20%	30%	40%	50%	60%	70%	80%	90%
Micro-F1	GF	79.63	80.51	80.94	81.18	81.38	81.54	81.63	81.71	81.78
	DeepWalk	78.89	79.92	80.41	80.69	80.92	81.08	81.21	81.35	81.42
	SkipGram	79.84	80.82	81.28	81.57	81.71	81.87	81.98	82.05	82.09
	LINE-SGD(1st)	76.03	77.05	77.57	77.85	78.08	78.25	78.39	78.44	78.49
	LINE-SGD(2nd)	74.68	76.53	77.54	78.18	78.63	78.96	79.19	79.40	79.57
	LINE(1st)	79.67	80.55	80.94	81.24	81.40	81.52	81.61	81.69	81.67
	LINE(2nd)	79.93	80.90	81.31	81.63	81.80	81.91	82.00	82.11	82.17
	LINE(1st+2nd)	**81.04****	**82.08****	**82.58****	**82.93****	**83.16****	**83.37****	**83.52****	**83.63****	**83.74****
Macro-F1	GF	79.49	80.39	80.82	81.08	81.26	81.40	81.52	81.61	81.68
	DeepWalk	78.78	79.78	80.30	80.56	80.82	80.97	81.11	81.24	81.32
	SkipGram	79.74	80.71	81.15	81.46	81.63	81.78	81.88	81.98	82.01
	LINE-SGD(1st)	75.85	76.90	77.40	77.71	77.94	78.12	78.24	78.29	78.36
	LINE-SGD(2nd)	74.70	76.45	77.43	78.09	78.53	78.83	79.08	79.29	79.46
	LINE(1st)	79.54	80.44	80.82	81.13	81.29	81.43	81.51	81.60	81.59
	LINE(2nd)	79.82	80.81	81.22	81.52	81.71	81.82	81.92	82.00	82.07
	LINE(1st+2nd)	**80.94****	**81.99****	**82.49****	**82.83****	**83.07****	**83.29****	**83.42****	**83.55****	**83.66****

Significantly outperforms GF at the: ** 0.01 and * 0.05 level, paired t-test.

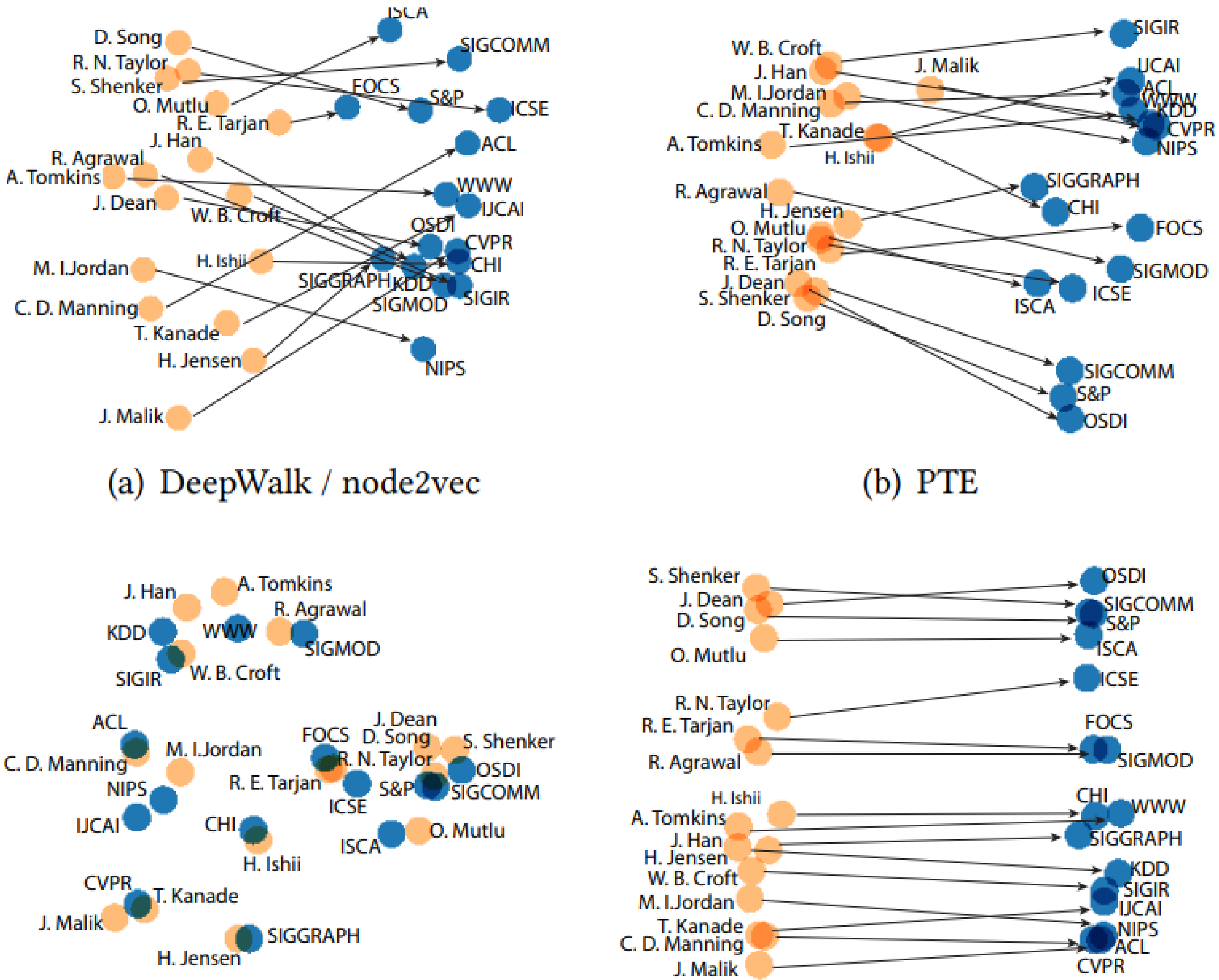
LINE



(a) GF (b) DeepWalk (c) LINE(2nd)

Figure 2: Visualization of the co-author network. The authors are mapped to the 2-D space using the t-SNE package with learned embeddings as input. Color of a node indicates the community of the author. Red: "data Mining," blue: "machine learning," green: "computer vision."

metapath2vec



(a) DeepWalk / node2vec (b) PTE

(c) *metapath2vec* (d) *metapath2vec++*

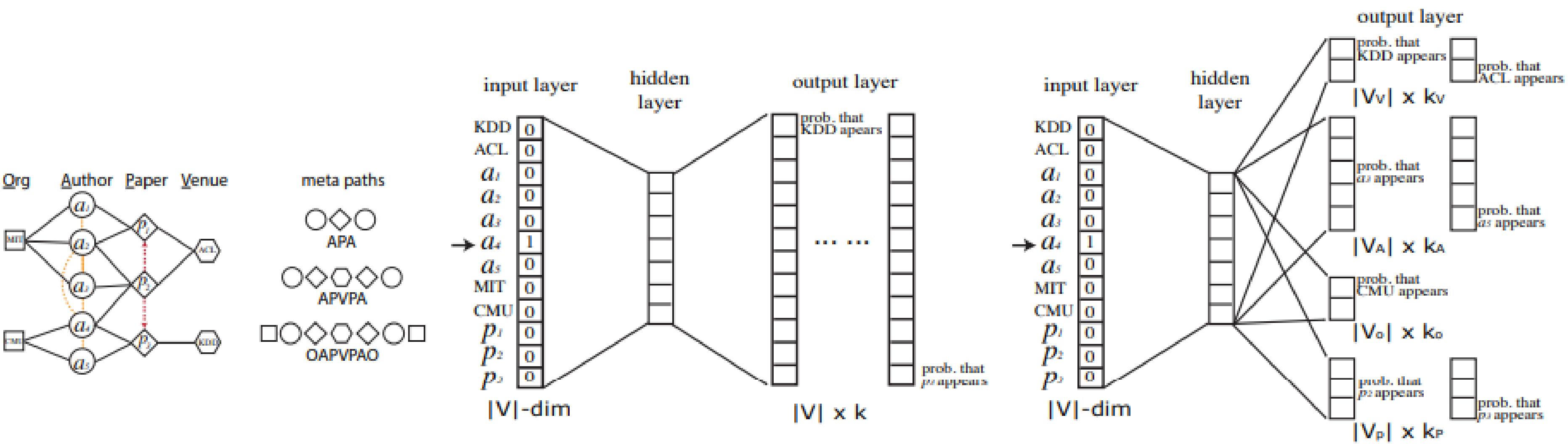
metapath2vec

- consider the nature of multi-typed node & entities

META PATH EXAMPLES AND THEIR PHYSICAL MEANINGS ON BIBLIOGRAPHIC DATA.

Path instance	Meta path	Physical meaning
Sun-NetClus-Han Sun-PathSim-Yu	Author-Paper-Author (*APA*)	Authors collaborate on the same paper
Sun-PathSim-VLDB-PathSim-Han Sun-PathSim-VLDB-GenClus-Aggarwal	Author-Paper-Venue-Paper-Author (*APVPA*)	Authors publish papers on the same venue
Sun-NetClus-KDD Sun-PathSim-VLDB	Author-Paper-Venue (*APV*)	Authors publish papers at a venue

Metapath2vec



(a) An academic network (b) Skip-gram in *metapath2vec*, node2vec, & DeepWalk (c) Skip-gram in *metapath2vec++*

Metapath2vec

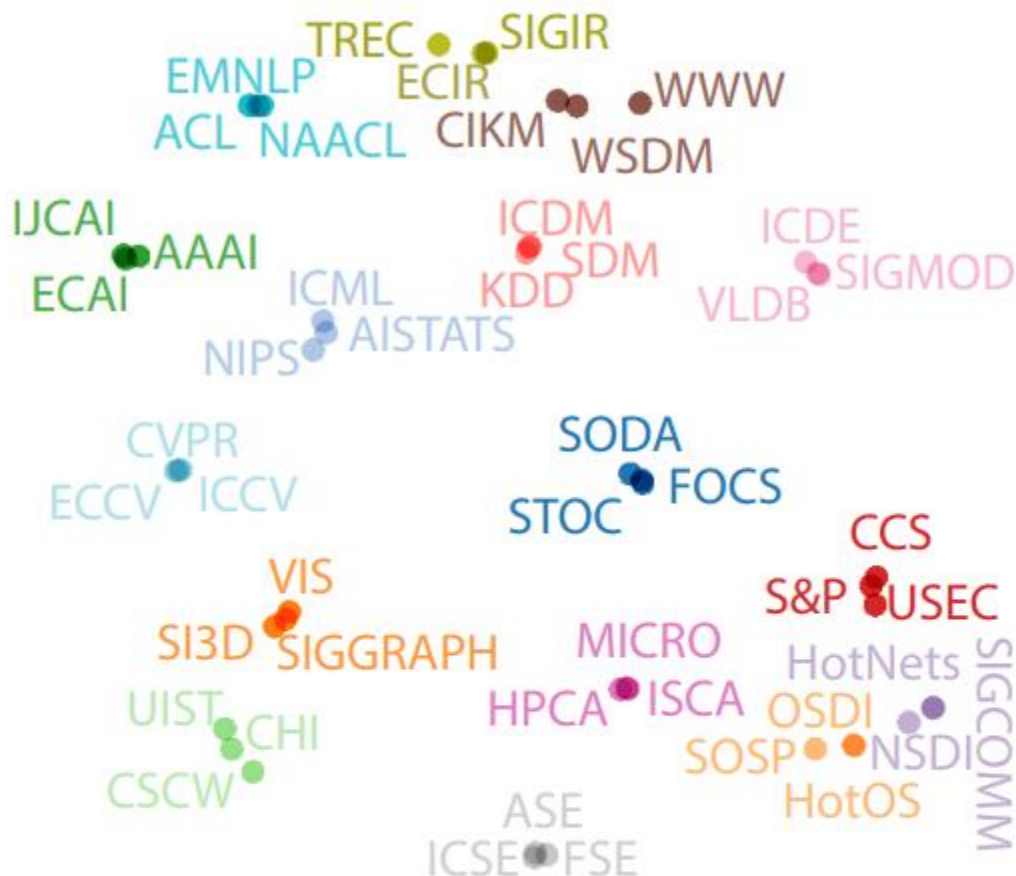


Table 2: Multi-class venue node classification results in AMiner data.

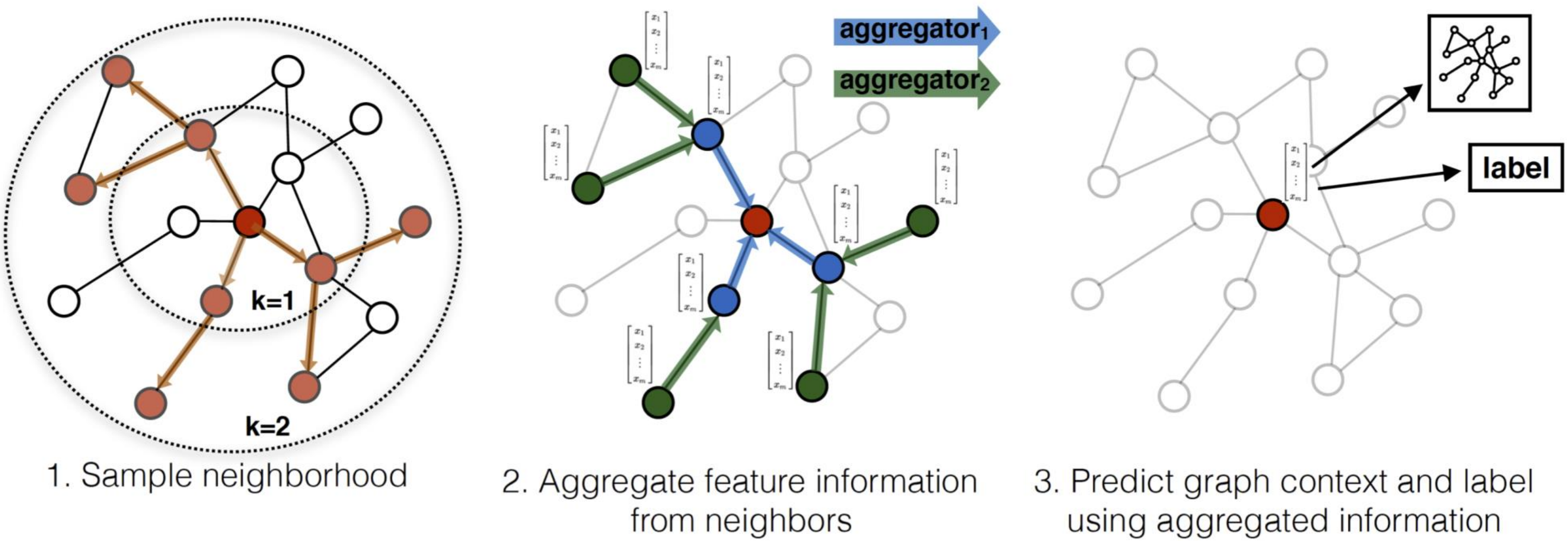
Metric	Method	5%	10%	20%	30%	40%	50%	60%	70%	80%	90%
Macro-F1	DeepWalk/node2vec	0.0723	0.1396	0.1905	0.2795	0.3427	0.3911	0.4424	0.4774	0.4955	0.4457
	LINE (1st+2nd)	0.2245	0.4629	0.7011	0.8473	0.8953	0.9203	0.9308	0.9466	0.9410	0.9466
	PTE	0.1702	0.3388	0.6535	0.8304	0.8936	0.9210	0.9352	0.9505	0.9525	0.9489
	metapath2vec	0.3033	0.5247	0.8033	0.8971	0.9406	0.9532	0.9529	0.9701	0.9683	0.9670
	metapath2vec++	0.3090	0.5444	0.8049	0.8995	0.9468	0.9580	0.9561	0.9675	0.9533	0.9503
Micro-F1	DeepWalk/node2vec	0.1701	0.2142	0.2486	0.3266	0.3788	0.4090	0.4630	0.4975	0.5259	0.5286
	LINE (1st+2nd)	0.3000	0.5167	0.7159	0.8457	0.8950	0.9209	0.9333	0.9500	0.9556	0.9571
	PTE	0.2512	0.4267	0.6879	0.8372	0.8950	0.9239	0.9352	0.9550	0.9667	0.9571
	metapath2vec	0.4173	0.5975	0.8327	0.9011	0.9400	0.9522	0.9537	0.9725	0.9815	0.9857
	metapath2vec++	0.4331	0.6192	0.8336	0.9032	0.9463	0.9582	0.9574	0.9700	0.9741	0.9786

Table 3: Multi-class author node classification results in AMiner data.

Metric	Method	5%	10%	20%	30%	40%	50%	60%	70%	80%	90%
Macro-F1	DeepWalk/node2vec	0.7153	0.7222	0.7256	0.7270	0.7273	0.7274	0.7273	0.7271	0.7275	0.7275
	LINE (1st+2nd)	0.8849	0.8886	0.8911	0.8921	0.8926	0.8929	0.8934	0.8936	0.8938	0.8934
	PTE	0.8898	0.8940	0.897	0.8982	0.8987	0.8990	0.8997	0.8999	0.9002	0.9005
	metapath2vec	0.9216	0.9262	0.9292	0.9303	0.9309	0.9314	0.9315	0.9316	0.9319	0.9320
	metapath2vec++	0.9107	0.9156	0.9186	0.9199	0.9204	0.9207	0.9207	0.9208	0.9211	0.9212
Micro-F1	DeepWalk/node2vec	0.7312	0.7372	0.7402	0.7414	0.7418	0.7420	0.7419	0.7420	0.7425	0.7425
	LINE (1st+2nd)	0.8936	0.8969	0.8993	0.9002	0.9007	0.9010	0.9015	0.9016	0.9018	0.9017
	PTE	0.8986	0.9023	0.9051	0.9061	0.9066	0.9068	0.9075	0.9077	0.9079	0.9082
	metapath2vec	0.9279	0.9319	0.9346	0.9356	0.9361	0.9365	0.9365	0.9365	0.9367	0.9369
	metapath2vec++	0.9173	0.9217	0.9243	0.9254	0.9259	0.9261	0.9261	0.9262	0.9264	0.9266

GraphSAGE

- Semi-supervised learning



GraphSAGE

Table 1: Prediction results for the three datasets (micro-averaged F1 scores). Results for unsupervised and fully supervised GraphSAGE are shown. Analogous trends hold for macro-averaged scores.

	Citation		Reddit		PPI	
Name	Unsup. F1	Sup. F1	Unsup. F1	Sup. F1	Unsup. F1	Sup. F1
Random	0.206	0.206	0.043	0.042	0.396	0.396
Raw features	0.575	0.575	0.585	0.585	0.422	0.422
DeepWalk	0.565	0.565	0.324	0.324	—	—
DeepWalk + features	0.701	0.701	0.691	0.691	—	—
GraphSAGE-GCN	0.742	0.772	**0.908**	0.930	0.465	0.500
GraphSAGE-mean	0.778	0.820	0.897	0.950	0.486	0.598
GraphSAGE-LSTM	0.788	0.832	**0.907**	**0.954**	0.482	**0.612**
GraphSAGE-pool	**0.798**	**0.839**	0.892	0.948	**0.502**	0.600
% gain over feat.	39%	46%	55%	63%	19%	45%

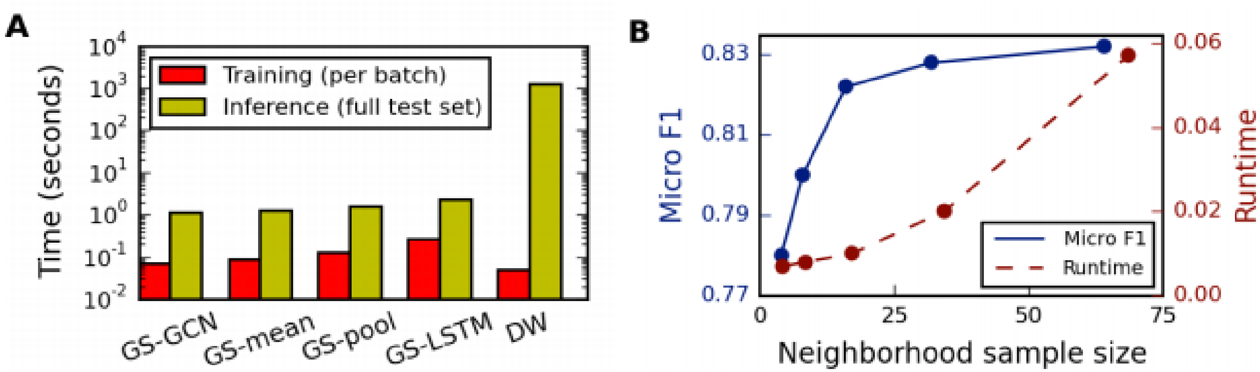


Figure 2: **A**: Timing experiments on Reddit data, with training batches of size 512 and inference on the full test set (79,534 nodes). **B**: Model performance with respect to the size of the sampled neighborhood, where the "neighborhood sample size" refers to the number of neighbors sampled at each depth for $K = 2$ with $S_1 = S_2$ (on the citation data using GraphSAGE-mean).