

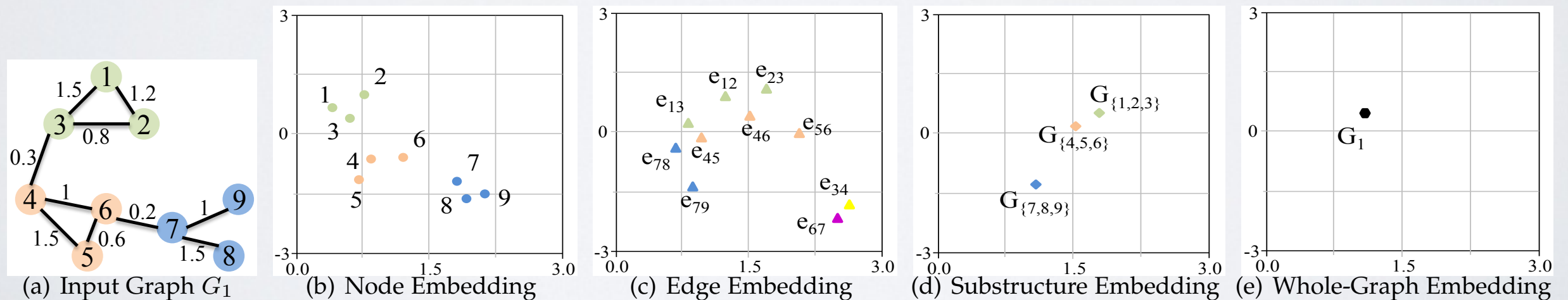
# GRAPH/NODE EMBEDDING

Goyal, P., & Ferrara, E. (2018). Graph embedding techniques, applications, and performance: A survey. *Knowledge-Based Systems*, 151, 78-94.

Cai, H., Zheng, V. W., & Chang, K. C. C. (2018). A comprehensive survey of graph embedding: Problems, techniques, and applications. *IEEE Transactions on Knowledge and Data Engineering*, 30(9), 1616-1637.

# VARIANT

- We can differentiate:
  - Node embedding
  - Edge Embedding
  - Substructure embedding
  - Whole graph Embedding
- In this course, only *node embedding* (often called graph embedding)



# NAMES

- Representation learning on networks
  - **Representation learning = feature learning**, as opposed to **manual feature engineering (heuristics)**
- Embedding  $\Rightarrow$  Latent space

# IN CONCRETE TERMS

- A graph is composed of
  - Nodes (possibly with labels)
  - Edges (possibly directed, weighted, with labels)
- A graph/node embedding technique in **d** dimensions will assign a vector of length **d** to each node, that will be useful for *\*what we want to do with the graph\**.
  - It captures some aspect of the network structure
- A vector can be assigned to an edge  $(u,v)$  by combining vectors of  $u$  and  $v$



# WHAT TO DO WITH EMBEDDINGS?

- Two possible ways to use an embedding:
  - Unsupervised learning:
    - The *distance* between vectors in the embedding is used for \*something\*
  - Supervised learning:
    - Algorithm learn to predict \*something\* from the features in the embedding

# WHAT CAN WE DO WITH EMBEDDINGS ?

# EMBEDDING TASKS

- Common tasks:
  - Link prediction (supervised)
  - Graph reconstruction (unsupervised link prediction ? / ad hoc)
  - Community detection (unsupervised)
  - Node classification (supervised community detection ?)
  - Role definition (Variant of node classification, can be unsupervised)
  - Visualisation (distances, like unsupervised)

# OVERVIEW OF MOST POPULAR METHODS



# PRE-DEEPWALK

MATRIX DECOMPOSITION

# LE: LAPLACIAN EIGENMAPS

- Introduced 2001
- Objective function:
  - $y^* = \min \sum_{i \neq j} \|y_i - y_j\|^2 S_{ij}$ 
    - $y^*$ : optimal embedding
    - $y_i$ : embedding of node  $i$
    - $S_{ij}$ : similarity between nodes  $i$  and  $j$  ( $A$ , heuristic, ...)
- Minimize the product between **distance in the embedding** and **similarity in the graph**
  - If nodes are *similar*, they must be *close* in the embedding

# LE: LAPLACIAN EIGENMAPS

- $y^* = \min \sum_{i \neq j} \|y_i - y_j\|^2 S_{ij}$

- ▶ Solution:  $d$  eigenvectors of lowest eigenvalues of  $D^{-1/2}LD^{-1/2}$
- ▶  $L$ : Laplacian, with  $S=A$

# HOPE: HIGHER-ORDER PROXIMITY PRESERVED EMBEDDING

- Preserve a proximity matrix

- $y^* = \min \sum_{i,j} |S_{ij} - y_i y_j^T|$

- $S$  can be the adjacency matrix, or number of common neighbors, Adamic Adar, etc.
- As similarity tends towards 0, embedding vectors must tend towards orthogonality (orthogonal vectors:  $y_i y_j^T = 0$ )



# LLE: LOCALLY LINEAR EMBEDDING

- Introduced 2000
- A node features can be represented as a linear combination of its neighbors'

$$y_i = \sum_j A_{ij} y_j$$

- Objective function:

$$y^* = \min \sum_i \|y_i - \sum_j A_{ij} y_j\|^2$$



# RANDOM WALKS BASED

# DEEPWALK

- The first *Random Walk+Neural Networks* graph embedding method.
  - First of a long series
- Adaptation of **word2vec/skipgram** to graphs

# SKIPGRAM

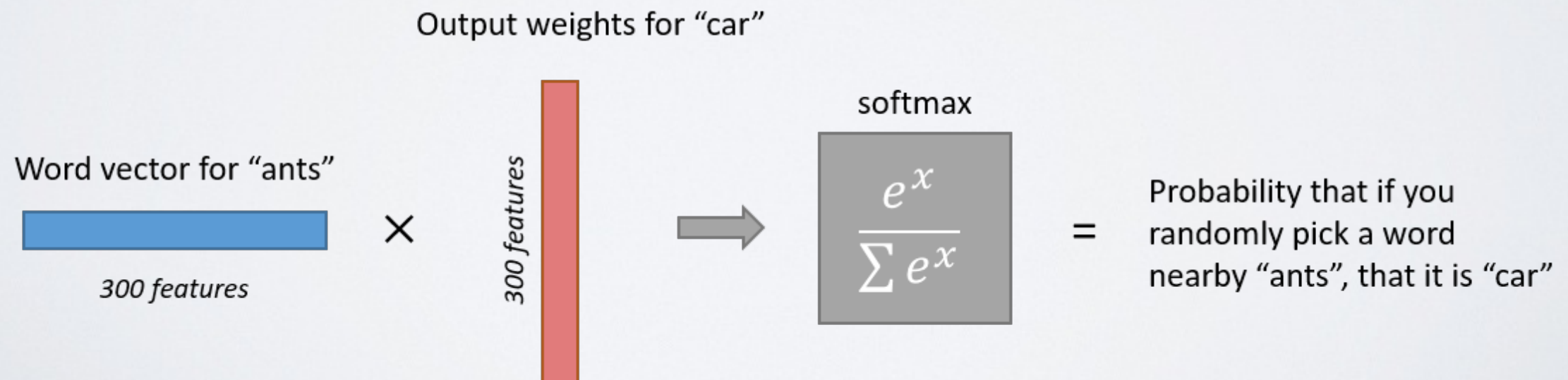
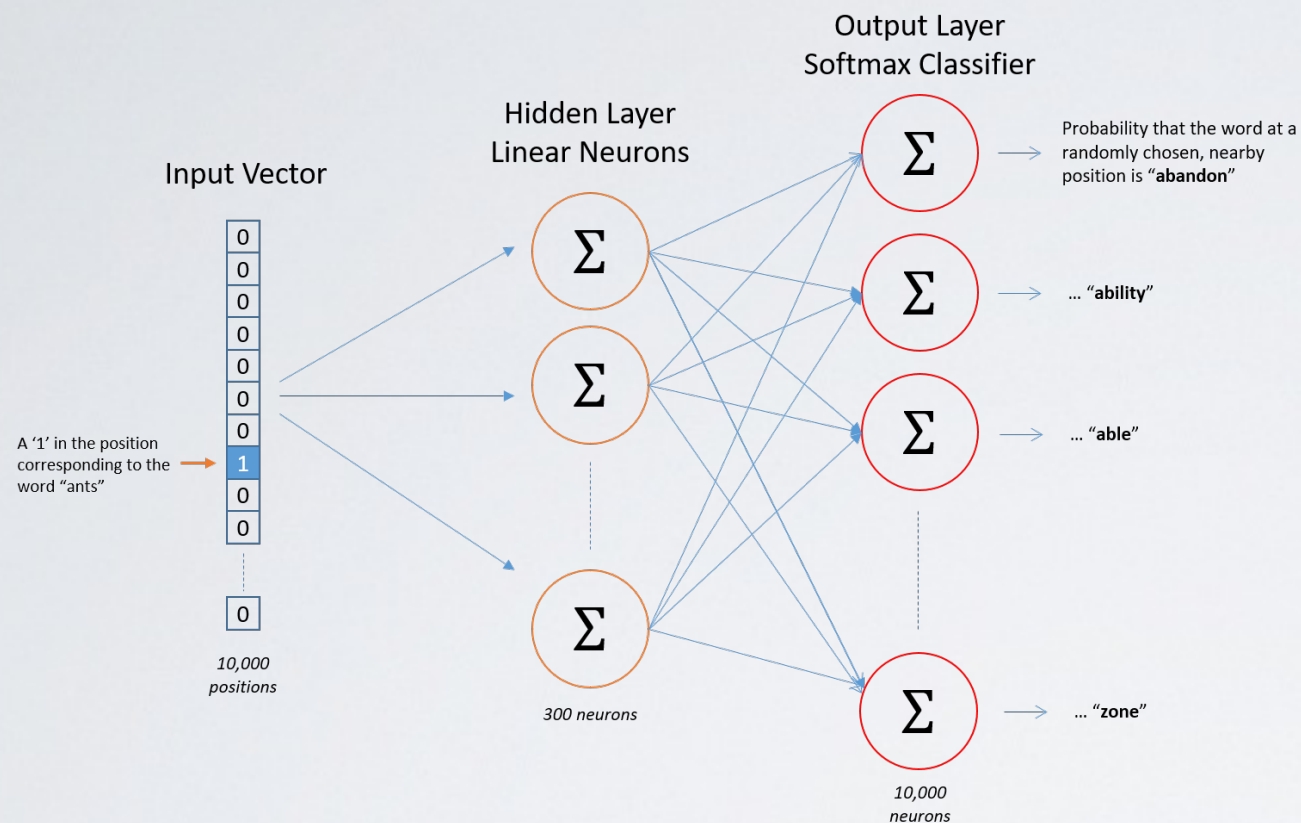
Word embedding

Corpus => Word = vectors

Similar embedding = similar **context**

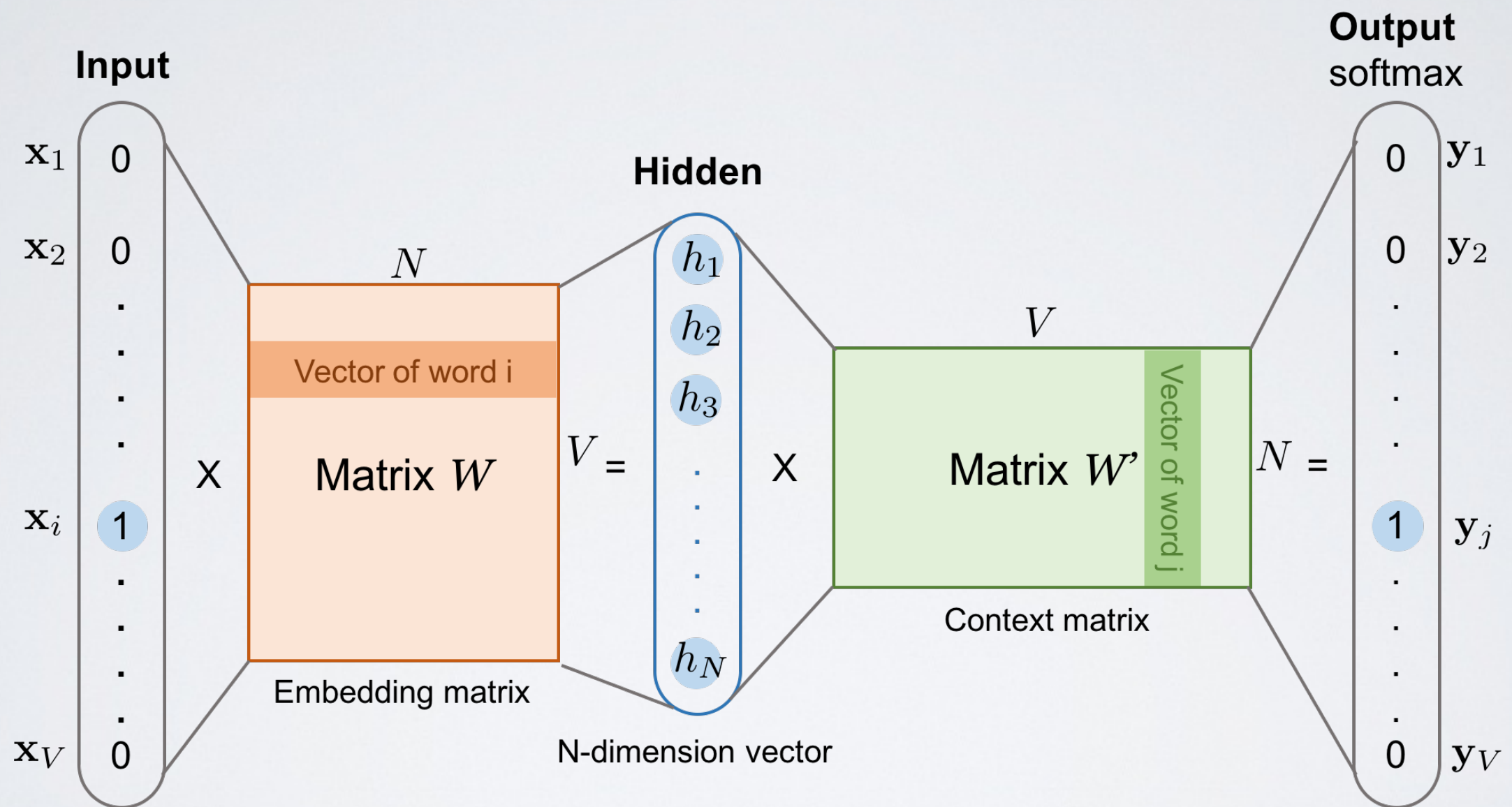
Source Text	Training Samples					
<table><tr><td>The</td><td>quick</td><td>brown</td></tr></table> fox jumps over the lazy dog. ➡	The	quick	brown	(the, quick) (the, brown)		
The	quick	brown				
<table><tr><td>The</td><td>quick</td><td>brown</td><td>fox</td></tr></table> jumps over the lazy dog. ➡	The	quick	brown	fox	(quick, the) (quick, brown) (quick, fox)	
The	quick	brown	fox			
<table><tr><td>The</td><td>quick</td><td>brown</td><td>fox</td><td>jumps</td></tr></table> over the lazy dog. ➡	The	quick	brown	fox	jumps	(brown, the) (brown, quick) (brown, fox) (brown, jumps)
The	quick	brown	fox	jumps		
The <table><tr><td>quick</td><td>brown</td><td>fox</td><td>jumps</td><td>over</td></tr></table> the lazy dog. ➡	quick	brown	fox	jumps	over	(fox, quick) (fox, brown) (fox, jumps) (fox, over)
quick	brown	fox	jumps	over		

# SKIPGRAM





# SKIPGRAM

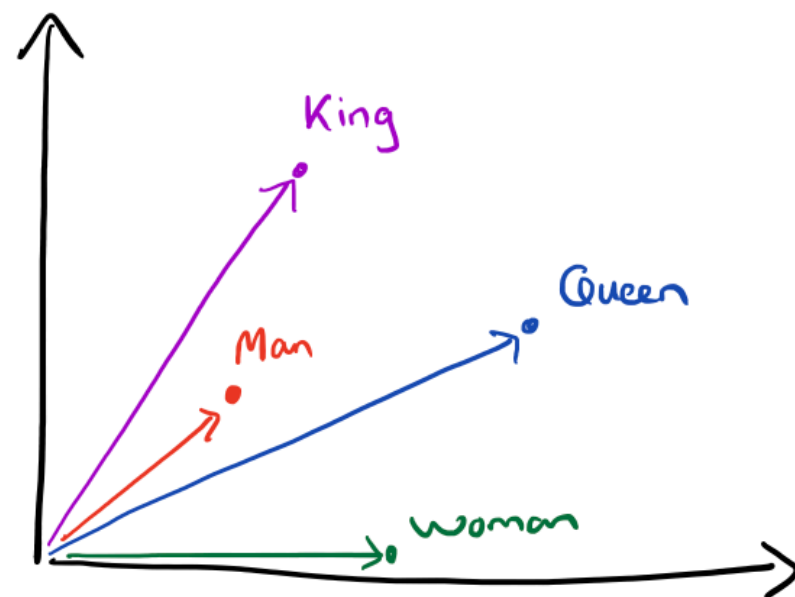


$\mathbf{N}$ =embedding size.  $\mathbf{V}$ =vocabulary size

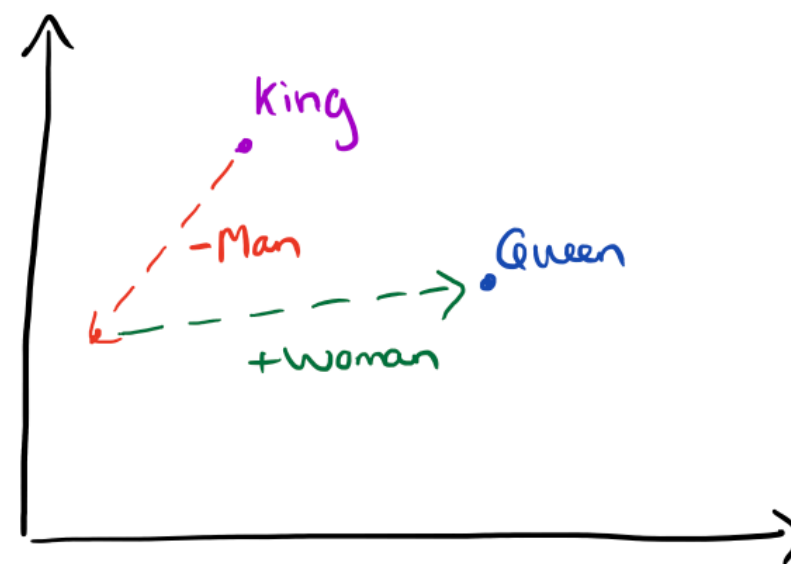


# SKIPGRAM

		King	Queen	Woman	Princess	...
Royalty		0.99	0.99	0.02	0.98	
Masculinity		0.99	0.05	0.01	0.02	
Femininity		0.05	0.93	0.999	0.94	
Age		0.7	0.6	0.5	0.1	
...		...				



Word  
Vectors



Vector  
Composition

[<https://blog.acolyer.org/2016/04/21/the-amazing-power-of-word-vectors/>]

# SKIPGRAM

Table 8: *Examples of the word pair relationships, using the best word vectors from Table 4 (Skip-gram model trained on 783M words with 300 dimensionality).*

Relationship	Example 1	Example 2	Example 3
France - Paris	Italy: Rome	Japan: Tokyo	Florida: Tallahassee
big - bigger	small: larger	cold: colder	quick: quicker
Miami - Florida	Baltimore: Maryland	Dallas: Texas	Kona: Hawaii
Einstein - scientist	Messi: midfielder	Mozart: violinist	Picasso: painter
Sarkozy - France	Berlusconi: Italy	Merkel: Germany	Koizumi: Japan
copper - Cu	zinc: Zn	gold: Au	uranium: plutonium
Berlusconi - Silvio	Sarkozy: Nicolas	Putin: Medvedev	Obama: Barack
Microsoft - Windows	Google: Android	IBM: Linux	Apple: iPhone
Microsoft - Ballmer	Google: Yahoo	IBM: McNealy	Apple: Jobs
Japan - sushi	Germany: bratwurst	France: tapas	USA: pizza

[<https://blog.acolyer.org/2016/04/21/the-amazing-power-of-word-vectors/>]

# GENERIC “SKIPGRAM”

- Algorithm that takes an input:
  - The element to embed
  - A list of “context” elements
- Provide as output:
  - An embedding with interesting properties
    - Works well for machine learning
    - Similar elements are close in the embedding
    - Somewhat preserves the overall structure

# DEEPWALK

- Skipgram for graphs:
  - 1)Generate “sentences” using random walks
  - 2)Apply Skipgram
- Parameters:
  - Embedding dimensions  $d$
  - Context size
  - More technical parameters: length of random walks, number of walks starting from each node, etc.



# NODE2VEC

- Use biased random walk to tune the context to capture \*what we want\*
  - “Breadth first” like RW => local neighborhood (edge probability ?)
  - “Depth-first” like RW => global structure ? (Communities ?)
  - 2 parameters to tune:
    - **p**: bias towards revisiting the previous node
    - **q**: bias towards exploring undiscovered parts of the network

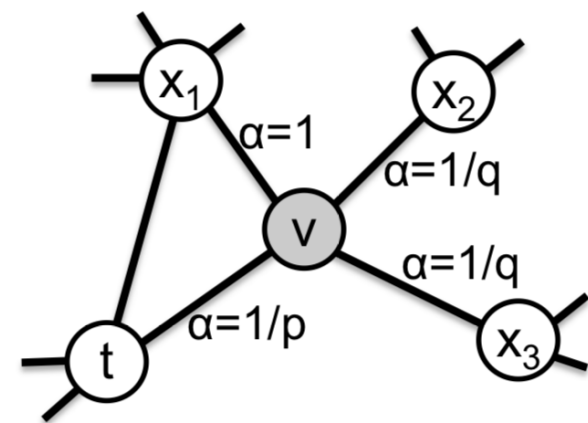


Figure 2: Illustration of the random walk procedure in *node2vec*. The walk just transitioned from  $t$  to  $v$  and is now evaluating its next step out of node  $v$ . Edge labels indicate search biases  $\alpha$ .



# RANDOM WALK METHODS

- What is the objective function ?
- How to interpret the distance between nodes in the embedding ?

# RANDOM WALK METHODS

Approximately

$$y = \min \sum_{(i,j)} p(n_j | n_i) - \sigma(y_i y_j^T)$$

with  $p(w_j | w_i)$  the probability to encounter node  $n_j$  in a random walk of a chosen length starting from node  $n_i$ . Its objective is therefore to make the distance in the embedding proportional to a random walk based distance in the graph.

with  $\sigma$  the softmax function defined as  $\frac{e^x}{\sum e^x}$ , a function commonly used in neural networks to add non-linearity and to ensure that the solution is a probability.

# RANDOM WALK METHODS

- Scalability:
  - Skipgram uses techniques from machine learning developed for very large datasets: highly **scalable** (not necessarily *fast* or *cost efficient*)
- Matrix factorization methods require the similarity matrix  $S$  as input
  - Computing all random walk distance:  $\mathcal{O}(n^2)$
  - $k$  random walks of length  $\ell$  from each node:  $\mathcal{O}(n)$

# ENCODER DECODER FRAMEWORK

Minimize a global loss defined as:

$$L = \sum_{(v_i, v_j) \in E} \ell(DEC(z_i, z_j), s_{\mathcal{G}}(v_i, v_j))$$

*DEC*: Decoder function (e.g.,  $DEC(z_i, z_j) = z_i^T z_j$ )

$s_{\mathcal{G}}$ : Ground truth similarity (e.g.,  $s_{\mathcal{G}}(v_i, v_j) = A_{ij}$ )

$\ell$ : Chosen loss function (e.g.,  $\ell(a, b) = |a - b|$ )



# ENCODER DECODER FRAMEWORK

Type	Method	Decoder	Proximity measure	Loss function ( $\ell$ )
Matrix factorization	Laplacian Eigenmaps [4]	$\ \mathbf{z}_i - \mathbf{z}_j\ _2^2$	general	$\text{DEC}(\mathbf{z}_i, \mathbf{z}_j) \cdot s_{\mathcal{G}}(v_i, v_j)$
	Graph Factorization [1]	$\mathbf{z}_i^\top \mathbf{z}_j$	$\mathbf{A}_{i,j}$	$\ \text{DEC}(\mathbf{z}_i, \mathbf{z}_j) - s_{\mathcal{G}}(v_i, v_j)\ _2^2$
	GraRep [9]	$\mathbf{z}_i^\top \mathbf{z}_j$	$\mathbf{A}_{i,j}, \mathbf{A}_{i,j}^2, \dots, \mathbf{A}_{i,j}^k$	$\ \text{DEC}(\mathbf{z}_i, \mathbf{z}_j) - s_{\mathcal{G}}(v_i, v_j)\ _2^2$
	HOPE [44]	$\mathbf{z}_i^\top \mathbf{z}_j$	general	$\ \text{DEC}(\mathbf{z}_i, \mathbf{z}_j) - s_{\mathcal{G}}(v_i, v_j)\ _2^2$
Random walk	DeepWalk [46]	$\frac{e^{\mathbf{z}_i^\top \mathbf{z}_j}}{\sum_{k \in \mathcal{V}} e^{\mathbf{z}_i^\top \mathbf{z}_k}}$	$p_{\mathcal{G}}(v_j   v_i)$	$-s_{\mathcal{G}}(v_i, v_j) \log(\text{DEC}(\mathbf{z}_i, \mathbf{z}_j))$
	node2vec [27]	$\frac{e^{\mathbf{z}_i^\top \mathbf{z}_j}}{\sum_{k \in \mathcal{V}} e^{\mathbf{z}_i^\top \mathbf{z}_k}}$	$p_{\mathcal{G}}(v_j   v_i)$ (biased)	$-s_{\mathcal{G}}(v_i, v_j) \log(\text{DEC}(\mathbf{z}_i, \mathbf{z}_j))$

$p_{\mathcal{G}}(v_j | v_i)$ : probability of visiting  $v_j$  on a fixed-length random walk started from  $v_i$



SOME REMARKS ON WHAT  
ARE EMBEDDINGS

# ADJACENCY MATRIX

- An adjacency matrix is an “embedding”... in high dimension
- That represents the structural equivalence
  - 2 nodes have similar “embeddings” if they have similar neighborhoods
  - Distance  $\Rightarrow$  # of different neighbors (Manhattan Distance)
- Standard dimensionality reduction (T-SNE, PCA) of this matrix?
  - Small dimensions
  - But still unintuitive notion of distance

# GRAPH LAYOUT

- Graph layouts are also embeddings.
  - Force layout, kamada-kawai ....
- They try to put connected nodes close to each other and non-connected ones “not close”
- Problem: they usually try to avoid overlaps
- Often not scalable

# NODE EMBEDDING: VISUALIZATION



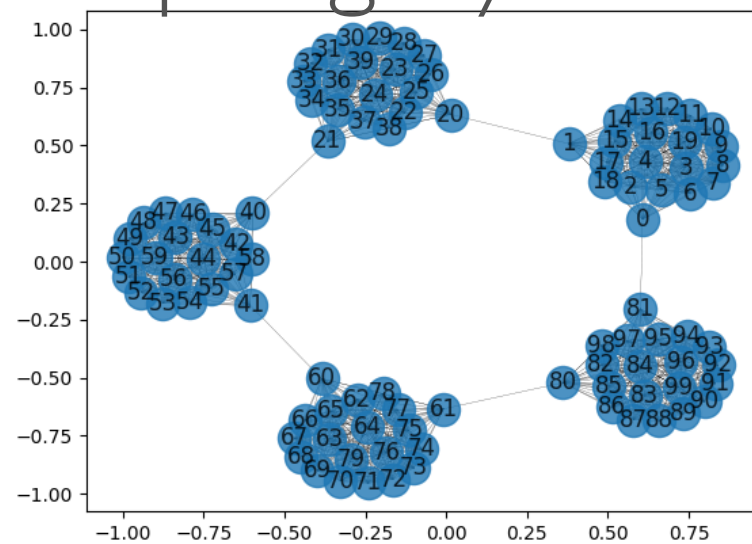
# FROM $D$ TO 2

- Graph embedding can be used to visualize graphs
- Requires to reduce the embedding from  $d$  to 2
  - TSNE
  - PCA
  - ...
- Interpretable positions of nodes
- But not necessarily optimized for human reading

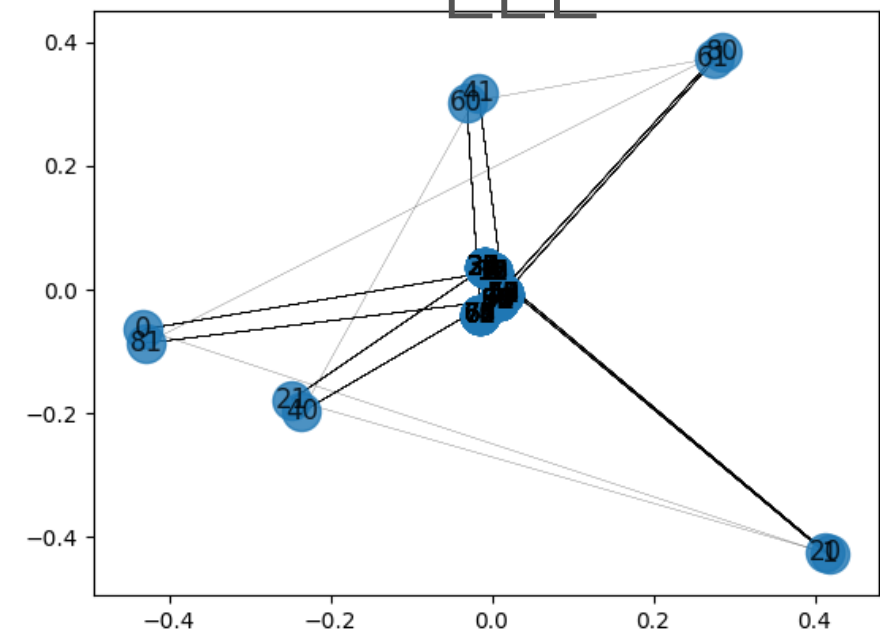
# CLIQUE RING

5 cliques of size 20 with 1 edge between them

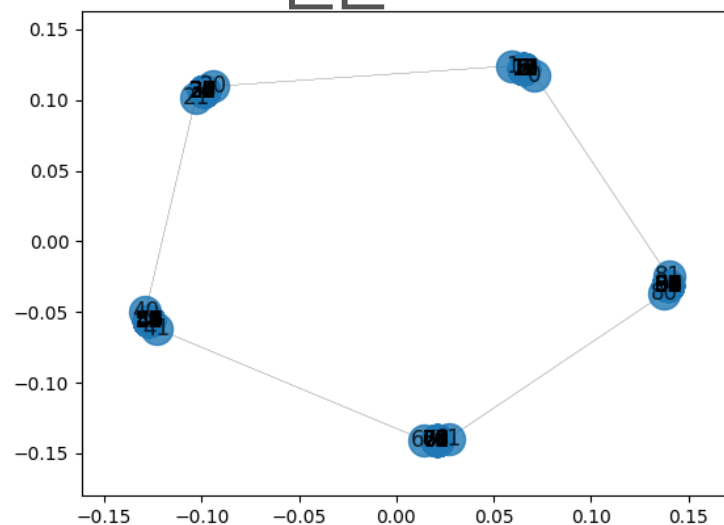
Spring layout



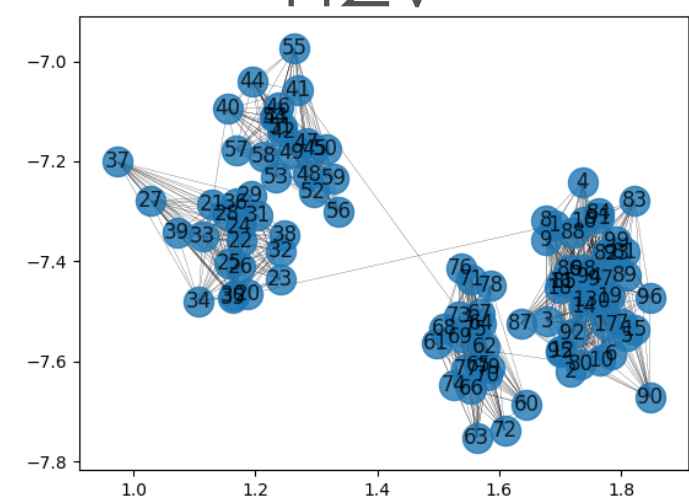
LLE



LE



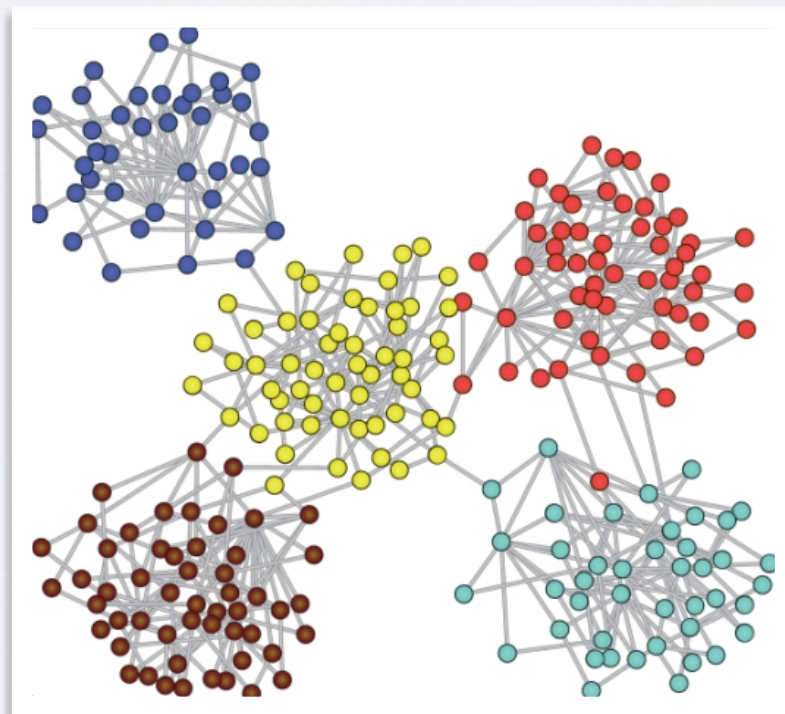
n2v



# NODE EMBEDDING: COMMUNITY DETECTION

# CLUSTERING EMBEDDINGS

- Many algorithm exists for **clustering** non-network data
  - K-means, DBscan, etc.
- Clustering: group nodes that are close in the feature space.



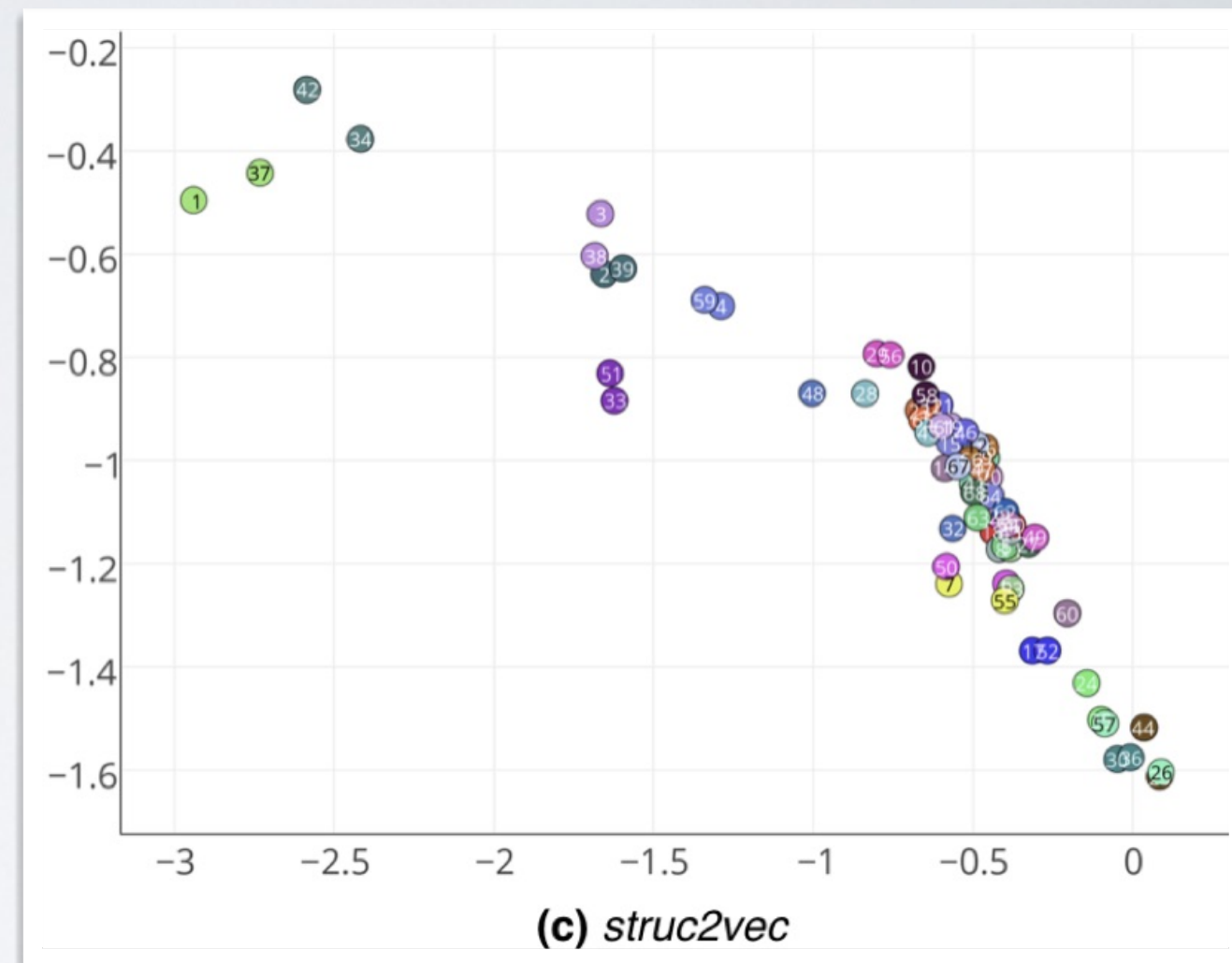
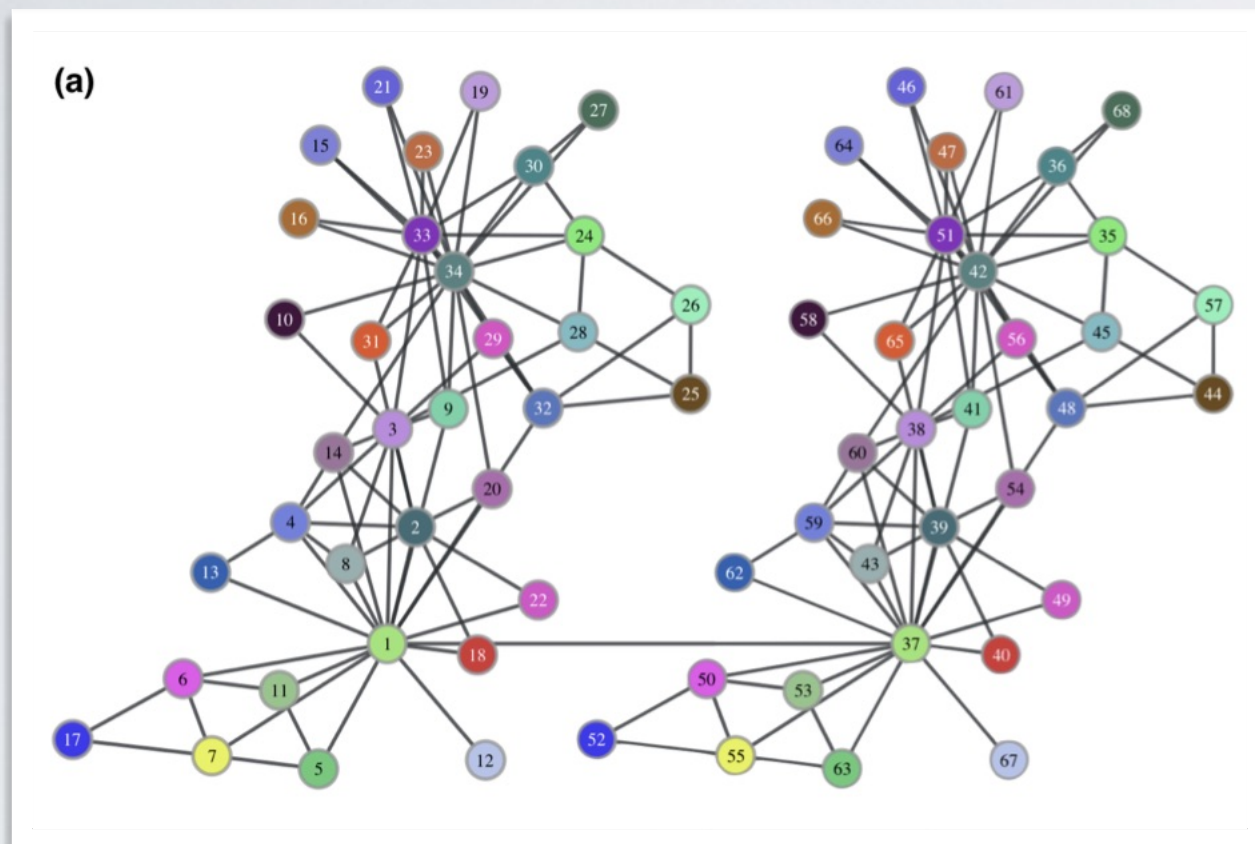


# EMBEDDING ROLES

# STRUC2VEC/ROLE2VEC

- In node2vec/Deepwalk, the context collected by RW contains the **labels** of encountered nodes
- Instead, we could memorize the **properties** of the nodes: attributes if available, or computed attributes (degrees, CC, ...)
- => Nodes with a same context will be nodes in a same “position” in the graph
- => Capture the role of nodes instead of proximity

# STRUCT2VEC : DOUBLE ZKC



# NODE CLASSIFICATION WITH EMBEDDINGS



# NODE CLASSIFICATION

- To each node is associated a vector in the embedding
  - This vector corresponds to topological features of the node, used instead of, for instance, centralities
  - Both types of features can be combined
- As usual, a classifier can be trained using those features

# NODE CLASSIFICATION

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
<i>node2vec</i>	<b>0.2581</b>	<b>0.1791</b>	<b>0.1552</b>
<i>node2vec</i> settings (p,q)	0.25, 0.25	4, 1	4, 0.5
<b>Gain of <i>node2vec</i> [%]</b>	<b>22.3</b>	<b>1.3</b>	<b>21.8</b>

Controversies...

# LINK PREDICTION WITH EMBEDDINGS

# UNSUPERVISED LINK PREDICTION

- Unsupervised link prediction **from embeddings**
- => Compute the distance between nodes in the embedding
- => Use it as a similarity score



# SUPERVISED LINK PREDICTION

- Supervised link prediction **from embeddings**
- $\Rightarrow$  embeddings provide features for nodes (nb features: dimensions)
  - Combine nodes features to obtain edge features
- $\Rightarrow$  Train a classifier to predict edges based on features from the embedding

# SUPERVISED LINK PREDICTION

Operator	Result
Average	$(\mathbf{a} + \mathbf{b})/2$
Concat	$[\mathbf{a}_1, \dots, \mathbf{a}_d, \mathbf{b}_1, \dots, \mathbf{b}_d]$
Hadamard	$[\mathbf{a}_1 * \mathbf{b}_1, \dots, \mathbf{a}_d * \mathbf{b}_d]$
Weighted L1	$[ \mathbf{a}_1 - \mathbf{b}_1 , \dots,  \mathbf{a}_d - \mathbf{b}_d ]$
Weighted L2	$[(\mathbf{a}_1 - \mathbf{b}_1)^2, \dots, (\mathbf{a}_d - \mathbf{b}_d)^2]$

Combining nodes vectors into edge vectors

# SUPERVISED LINK PREDICTION

- How well does it work ?
- According to creators articles
  - Node2vec (2016)
  - VERSE (2018)
- => These methods are better than the state of the art

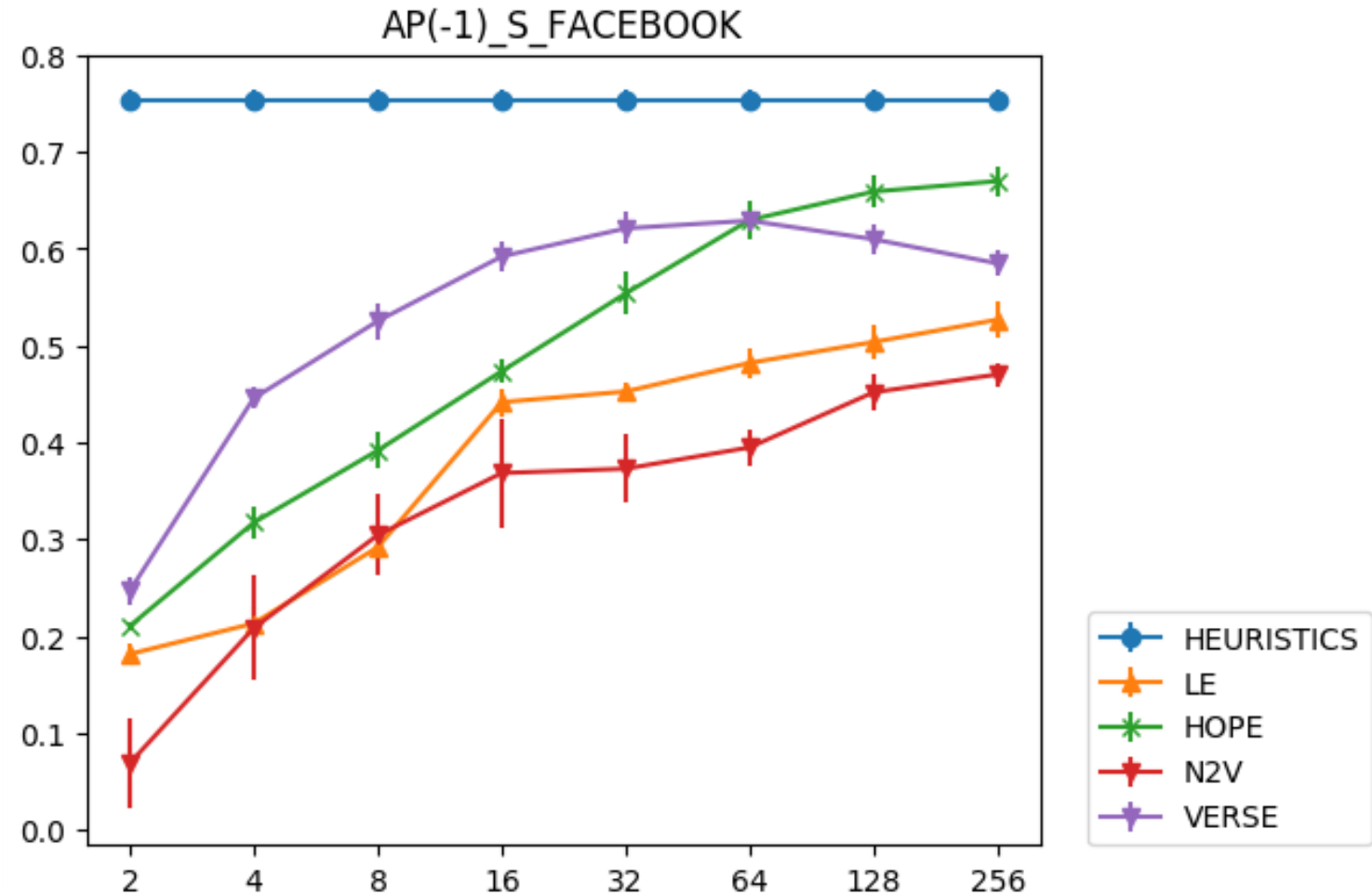
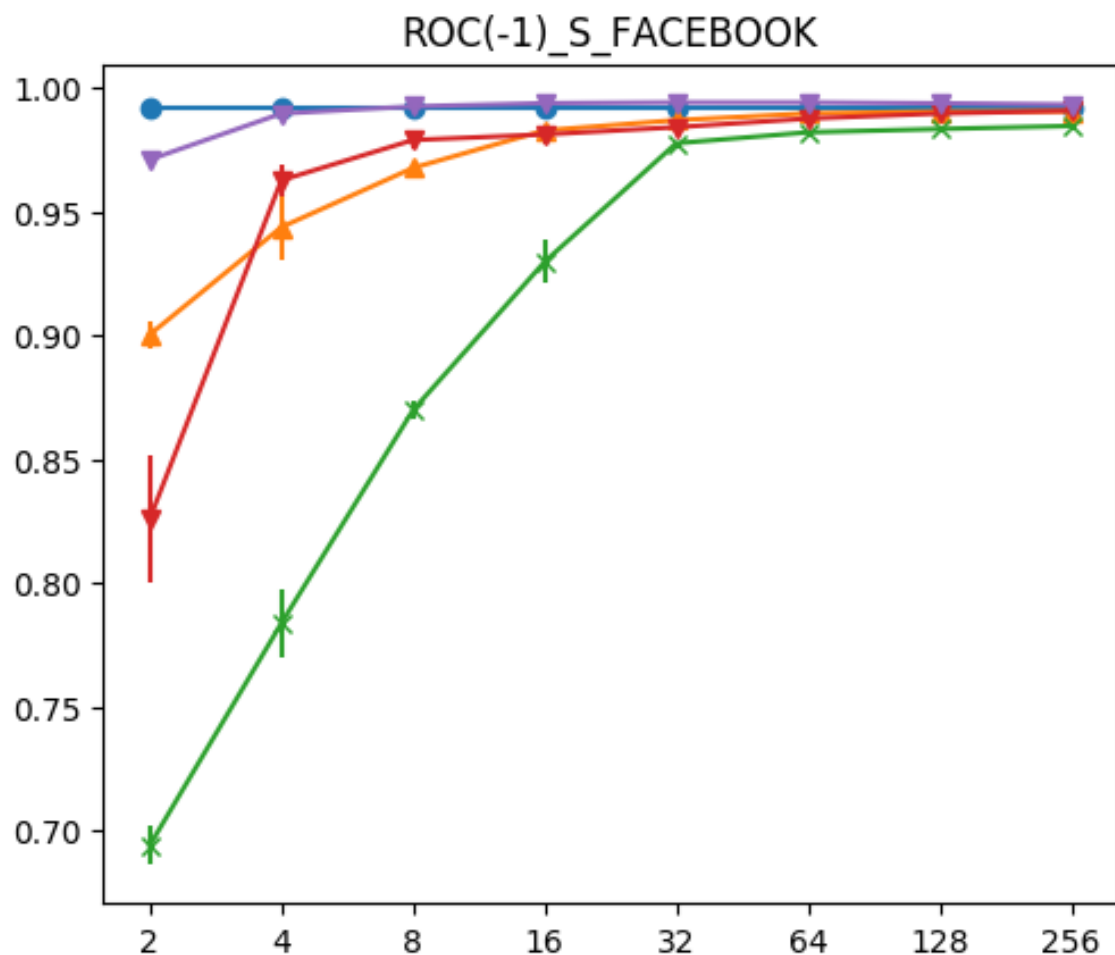
Op	Algorithm	Dataset		
		Facebook	PPI	arXiv
	Common Neighbors	0.8100	0.7142	0.8153
	Jaccard's Coefficient	0.8880	0.7018	0.8067
	Adamic-Adar	0.8289	0.7126	0.8315
	Pref. Attachment	0.7137	0.6670	0.6996
(a)	Spectral Clustering	0.5960	0.6588	0.5812
	DeepWalk	0.7238	0.6923	0.7066
	LINE	0.7029	0.6330	0.6516
	<i>node2vec</i>	0.7266	0.7543	0.7221
(b)	Spectral Clustering	0.6192	0.4920	0.5740
	DeepWalk	<b>0.9680</b>	0.7441	0.9340
	LINE	0.9490	0.7249	0.8902
	<i>node2vec</i>	<b>0.9680</b>	<b>0.7719</b>	<b>0.9366</b>
(c)	Spectral Clustering	0.7200	0.6356	0.7099
	DeepWalk	0.9574	0.6026	0.8282
	LINE	0.9483	0.7024	0.8809
	<i>node2vec</i>	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
	<i>node2vec</i>	0.9606	0.6236	0.8477

(a) Average, (b) Hadamard, (c) Weighted-L1, and (d) Weighted-L2

(AUC)

# LINK PREDICTION

- Personal opinion: not that simple

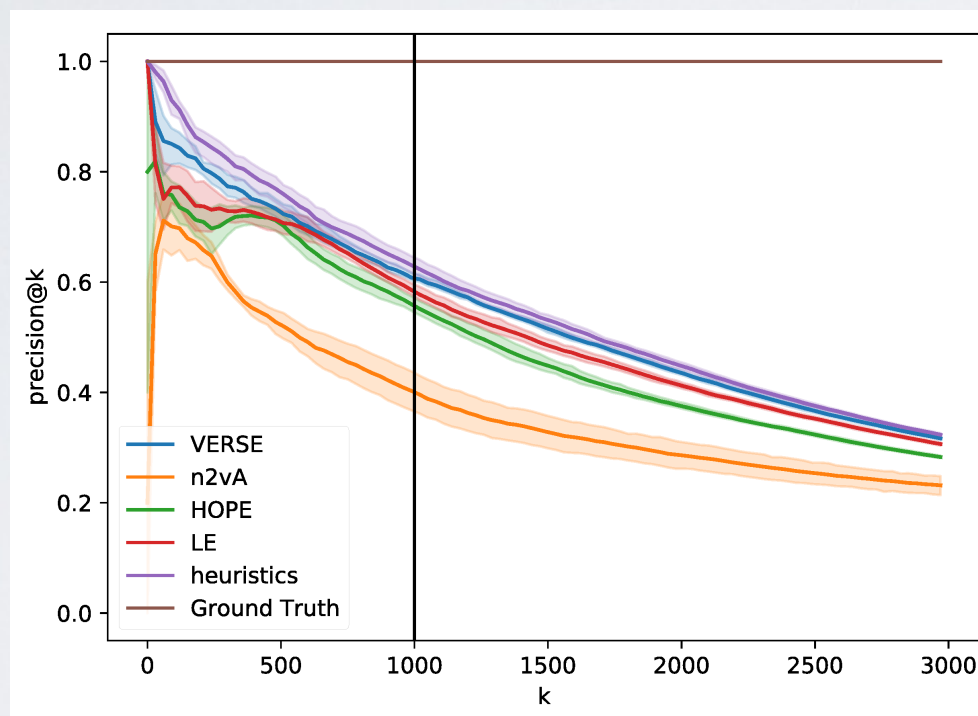




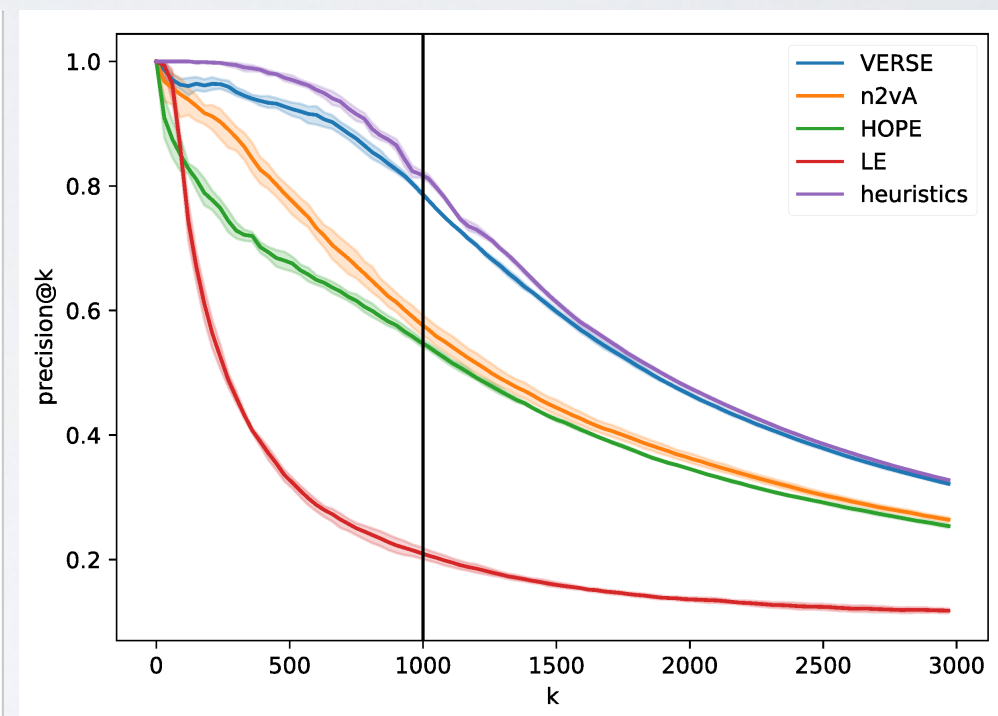
# LINK PREDICTION

- First few predictions: advantage to heuristics

Better prediction at distance 2, worst otherwise



(a) FACEBOOK



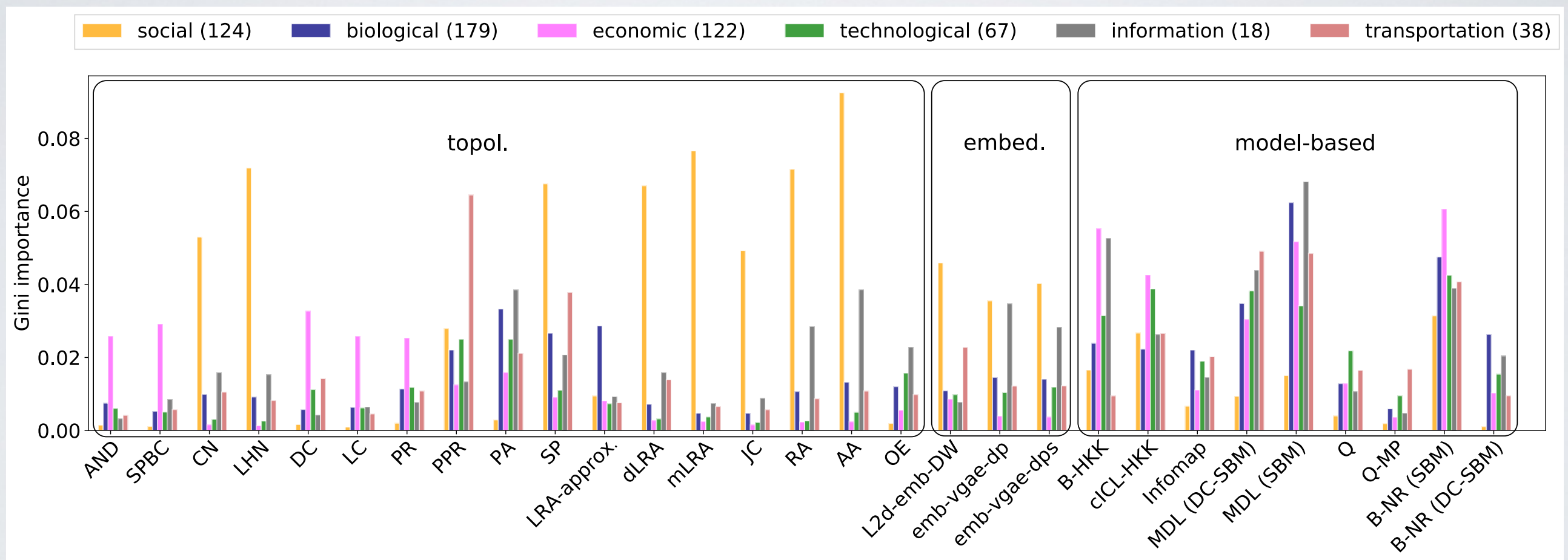
(b) ASTROPH

# MODEL STACKING

FOR LINK PREDICTION

# MODEL STACKING

Ghasemian, A., Hosseinmardi, H., Galstyan, A., Airolidi, E. M., & Clauset, A. (2020). Stacking models for nearly optimal link prediction in complex networks. *Proceedings of the National Academy of Sciences*, 117(38), 23393-23400.



# MODEL STACKING

**Table S12.** Average AUC, precision, and recall performances of the link prediction algorithms over 124 social networks as a subset of CommunityFitNet corpus. A random forest is used for supervised stacking of methods. Here, the predictors are adjusted for maximum F measure using a model selection through a cross validation on training set. The results are reported on 20% holdout test set.

Algorithm	AUC	Precision	Recall
Q	0.89 ± 0.07	0.42 ± 0.13	0.85 ± 0.08
Q-MR	0.87 ± 0.07	0.38 ± 0.16	0.78 ± 0.07
Q-MP	0.86 ± 0.08	0.25 ± 0.07	0.83 ± 0.09
B-NR (SBM)	0.93 ± 0.06	0.3 ± 0.08	0.85 ± 0.12
B-NR (DC-SBM)	0.93 ± 0.07	0.28 ± 0.08	0.88 ± 0.08
cICL-HKK	0.93 ± 0.08	0.34 ± 0.1	0.85 ± 0.14
B-HKK	0.88 ± 0.07	0.17 ± 0.05	0.79 ± 0.17
Infomap	0.91 ± 0.04	0.29 ± 0.08	0.83 ± 0.05
MDL (SBM)	0.94 ± 0.07	0.31 ± 0.09	0.87 ± 0.16
MDL (DC-SBM)	0.93 ± 0.09	0.26 ± 0.09	0.89 ± 0.11
S-NB	0.94 ± 0.07	0.3 ± 0.1	0.87 ± 0.08
mean model-based	0.91 ± 0.08	0.3 ± 0.12	0.84 ± 0.12
mean indiv. topol.	0.64 ± 0.19	0.2 ± 0.27	0.56 ± 0.33
mean indiv. topol. & model	0.7 ± 0.21	0.22 ± 0.25	0.62 ± 0.32
emd-DW	0.95 ± 0.1	0.45 ± 0.16	0.92 ± 0.13
emb-vgae	0.95 ± 0.08	0.09 ± 0.02	0.96 ± 0.09
all topol.	0.97 ± 0.08	0.89 ± 0.21	0.88 ± 0.2
all model-based	0.95 ± 0.07	0.76 ± 0.2	0.68 ± 0.17
all embed.	0.95 ± 0.11	0.75 ± 0.23	0.74 ± 0.23
all topol. & model	0.98 ± 0.06	0.89 ± 0.22	0.88 ± 0.19
all topol. & embed.	0.96 ± 0.1	0.86 ± 0.22	0.83 ± 0.25
all model & embed.	0.96 ± 0.09	0.78 ± 0.21	0.74 ± 0.22
all topol., model & embed.	0.97 ± 0.09	0.86 ± 0.23	0.84 ± 0.23

**Table 1.** Link prediction performance (mean ± std. err.), measured by AUC, precision, and recall, for link prediction algorithms applied to the 548 structurally diverse networks in our corpus.

algorithm	AUC	precision	recall
Q	0.7 ± 0.14	0.14 ± 0.17	0.67 ± 0.15
Q-MR	0.67 ± 0.15	0.12 ± 0.17	0.63 ± 0.13
Q-MP	0.64 ± 0.15	0.09 ± 0.11	0.59 ± 0.17
B-NR (SBM)	0.81 ± 0.13	0.13 ± 0.12	0.65 ± 0.22
B-NR (DC-SBM)	0.7 ± 0.2	0.12 ± 0.12	0.61 ± 0.24
cICL-HKK	0.79 ± 0.13	0.14 ± 0.14	0.58 ± 0.25
B-HKK	0.77 ± 0.13	0.11 ± 0.1	0.51 ± 0.26
Infomap	0.73 ± 0.14	0.12 ± 0.12	0.68 ± 0.13
MDL (SBM)	0.79 ± 0.15	0.14 ± 0.13	0.57 ± 0.3
MDL (DC-SBM)	0.84 ± 0.1	0.13 ± 0.11	0.78 ± 0.12
S-NB	0.71 ± 0.19	0.12 ± 0.13	0.66 ± 0.17
mean model-based	0.74 ± 0.16	0.12 ± 0.13	0.63 ± 0.21
mean indiv. topol.	0.6 ± 0.13	0.09 ± 0.16	0.53 ± 0.35
mean indiv. topol. & model	0.63 ± 0.15	0.09 ± 0.16	0.55 ± 0.33
emb-DW	0.63 ± 0.23	0.17 ± 0.19	0.42 ± 0.35
emb-vgae	0.69 ± 0.19	0.05 ± 0.05	0.69 ± 0.21
all topol.	0.86 ± 0.11	0.42 ± 0.33	0.44 ± 0.32
all model-based	0.83 ± 0.12	0.39 ± 0.34	0.3 ± 0.29
all embed.	0.77 ± 0.16	0.32 ± 0.32	0.32 ± 0.31
all topol. & model	0.87 ± 0.1	0.48 ± 0.36	0.35 ± 0.35
all topol. & embed.	0.84 ± 0.13	0.4 ± 0.34	0.39 ± 0.33
all model & embed.	0.84 ± 0.13	0.36 ± 0.32	0.36 ± 0.31
all topol., model & embed.	0.85 ± 0.14	0.42 ± 0.34	0.39 ± 0.33