Scaling Attributed Network Embedding to Massive Graphs

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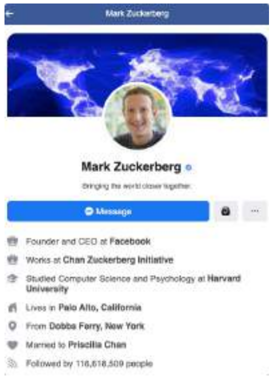
Yin Yang, Juncheng Liu, Sourav S. Bhowmick

Outline

- Problem Definition
- Applications
- Existing Work & Challenges
- Node-Attribute & Attribute-Node Affinity
- Objective Function & Solution
- Parallel Implementations
- Experiments

Attributed Network

- **Input**: a graph G, where each node u has some attributes from a set R, e.g., a social network user has an attribute "gender"



Mark Zuckerberg

Bringing the world closer together.

Founder and CEO at **Facebook**

Works at **Chan Zuckerberg Initiative**

Studied Computer Science and Psychology at **Harvard University**

Lives in **Palo Alto, California**

From **Dobbs Ferry, New York**

Married to **Priscilla Chan**

Followed by 116,618,509 people

Mark Zuckerberg

Gender: M
Country: USA
Age: 37
#fans: 116M

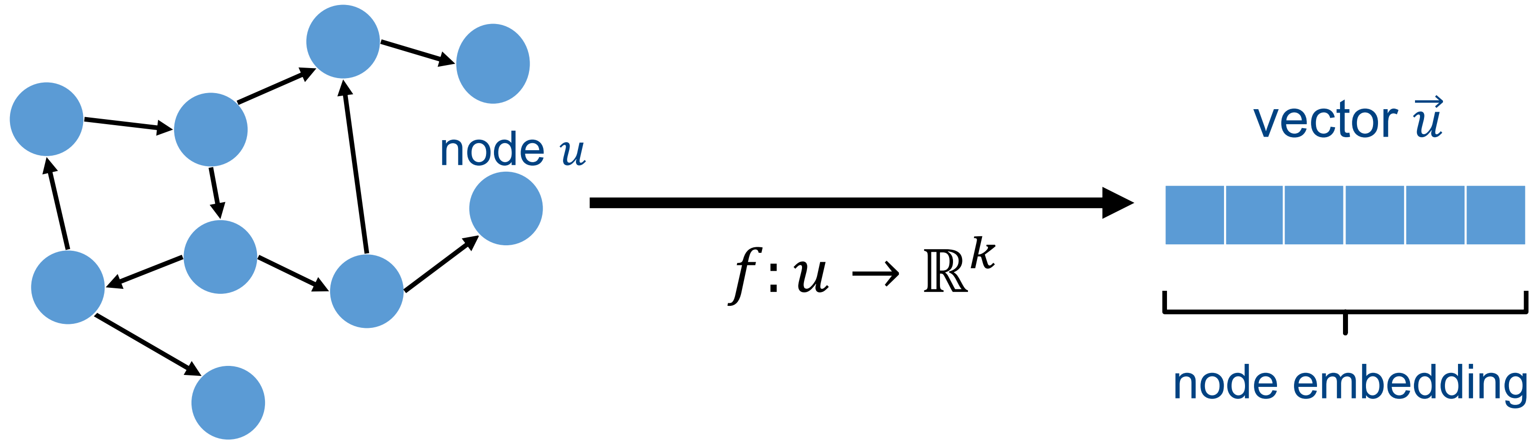
$\Rightarrow$

M: 1
F: 0
Other: 0

- Each node-attribute pair (u, r) has a weight $w(u, r)$ that indicates the strength of association

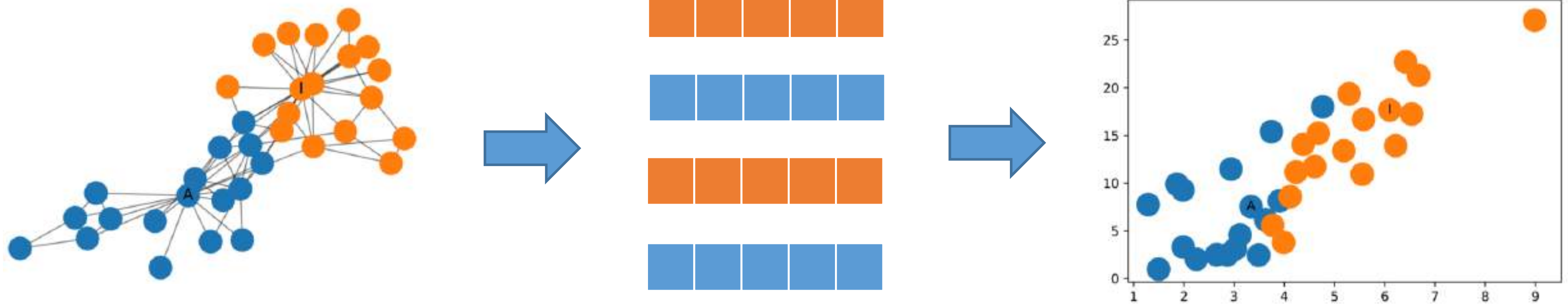
Attributed Network Embedding (ANE)

- **Objective**: Map each node to an embedding vector, which can then be used as input to downstream machine learning tasks



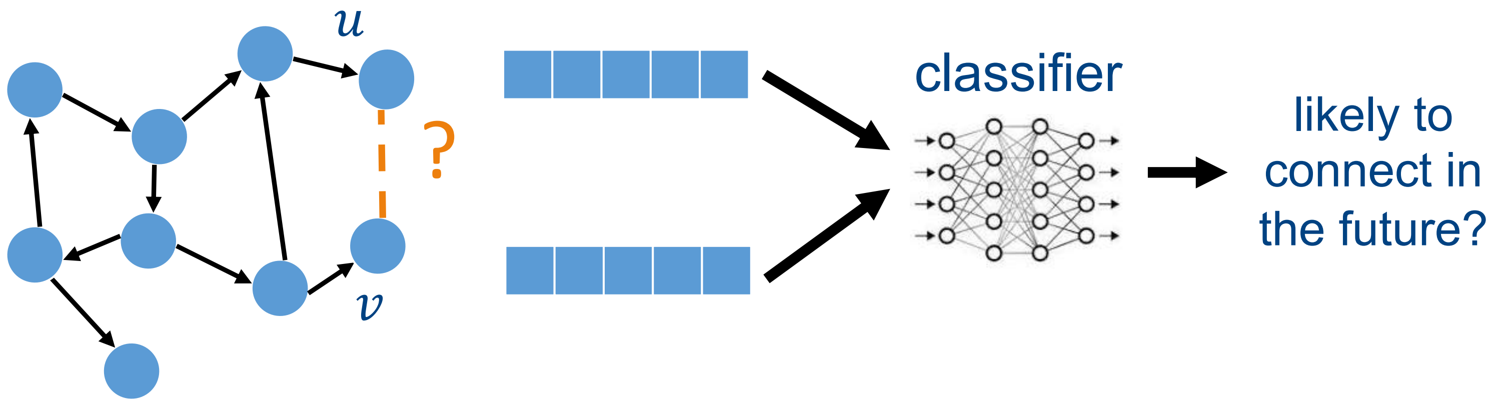
Applications

- Node classification
  - user tagging in social networks
  - fraud detection in financial networks
  - cancer biomarkers identification in biological networks



Applications

- Link Prediction
  - image/video recommendation in Pinterest [Ying KDD'18]
  - product recommendation in Alibaba [Cen KDD'19]

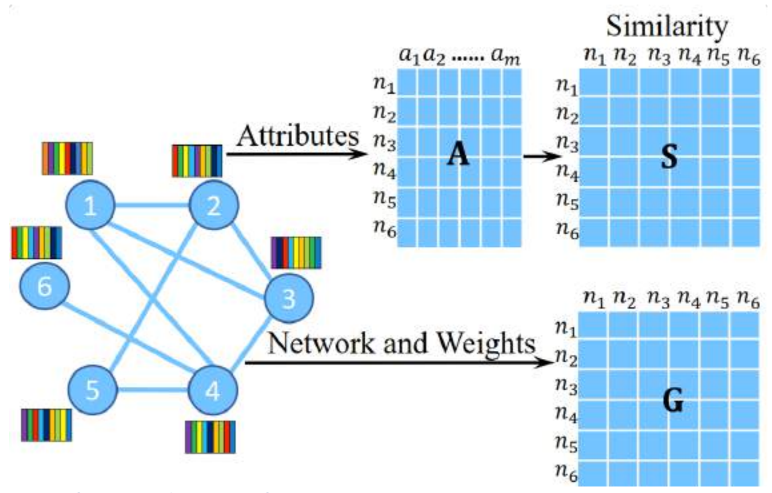


Ying et al. Graph Convolutional Neural Networks for Web-Scale Recommender Systems. KDD'18.

Cen et al. Representation Learning for Attributed Multiplex Heterogeneous Network. KDD'19.

Existing work

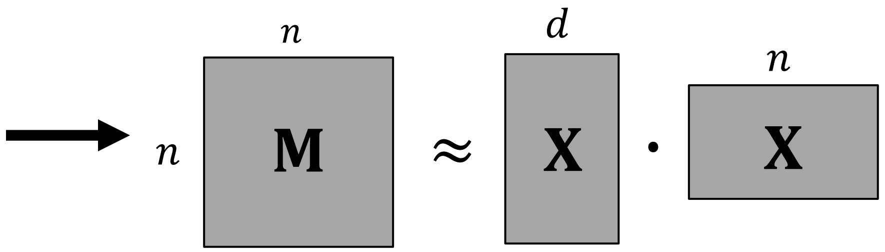
- Matrix Factorization-based methods


Attributes
$a_1 a_2 \ldots\ldots a_m$
n_1 n_2 n_3 n_4 n_5 n_6
A
Similarity
S
Network and Weights
G
1
2
3
4
5
6

attributed graph G

Affinity

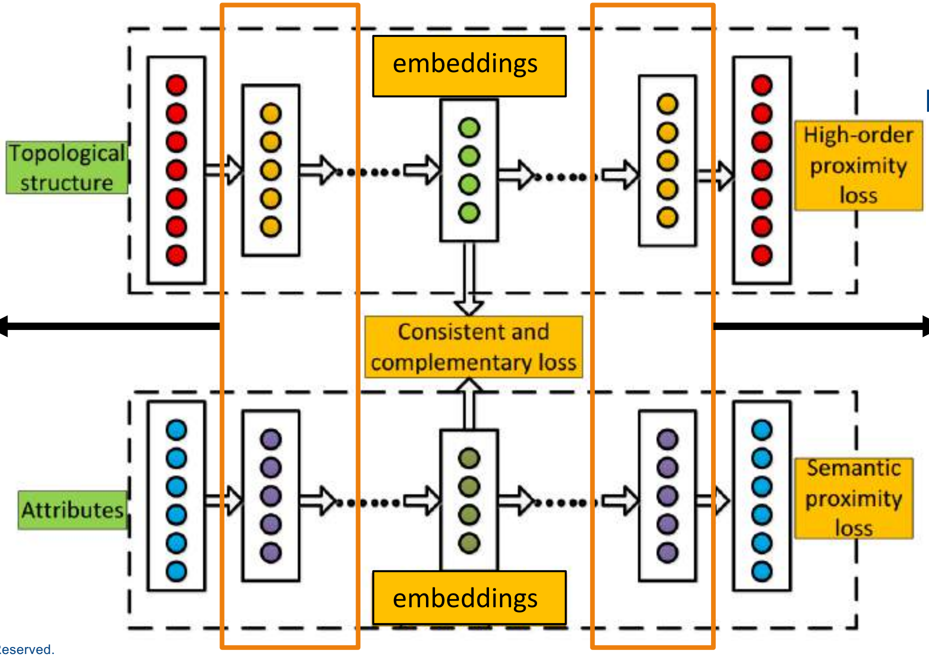
Factorize the combined matrix of $\boldsymbol{S}$ and $\mathbf{G}$



Existing work

- Neural networks-based methods

Encoders: neural networks that compress data into embeddings

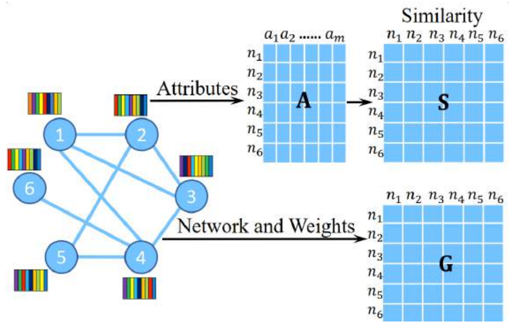


Minimize reconstruction loss

Decoders: neural networks that reconstruct input data from the embeddings

Limitations

- Existing ANE solutions
  - generate effective embeddings based on expensive learning techniques (e.g., auto-encoders). This makes them difficult to handle large graphs.
  - are more efficient but produce low-quality embeddings.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n_1 n_2 n_3 n_4 n_5 n_6
1
2
3
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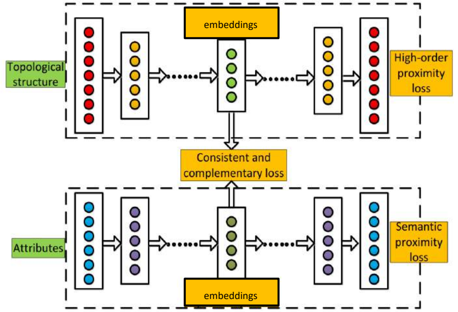
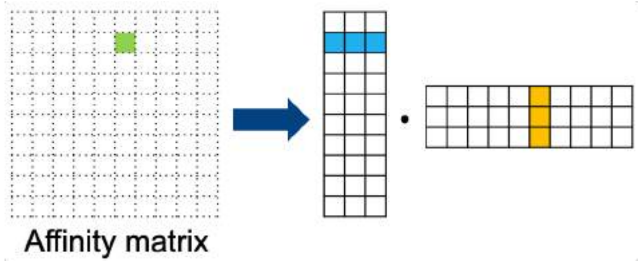


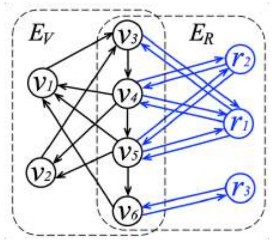
Basic idea & challenges

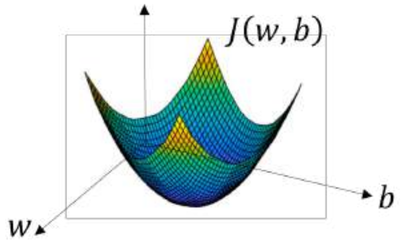
- Objective: Construct high-quality embeddings without significant computation cost
- Basic idea: formulate ANE as a new matrix factorization problem
- Challenges
  - Two types of affinity to capture: node-node & node-attribute
    - How to model these affinities?
    - How to compute & store these affinities? ($O(n^2)$ space, n=#nodes)
  - Two affinity matrices
    - Which one are we factorizing?
    - How to design the objective function?

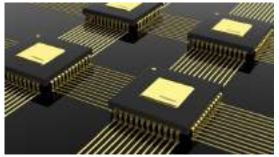


Solution Overview: PANE

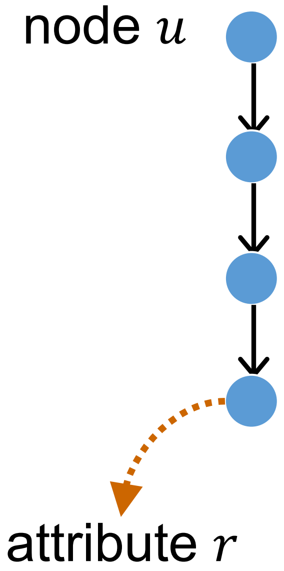
- Construct node-attribute affinity matrix $\mathbf{F}$ & attribute-node affinity matrix $\mathbf{B}$
  - forward & backward random walk models
  - indirectly model node-node affinity via $\mathbf{F}$ & $\mathbf{B}$
- Joint factorization of affinity matrices $\mathbf{F}$ & $\mathbf{B}$
  - initialize embeddings via singular value decomposition
- Parallelize PANE for higher efficiency
  - parallel singular value decomposition

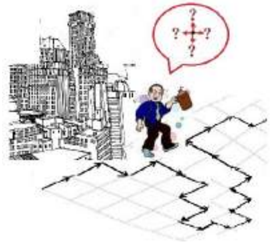


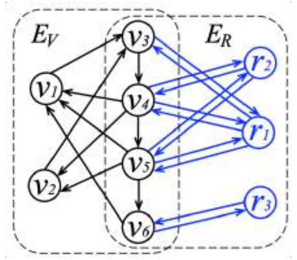


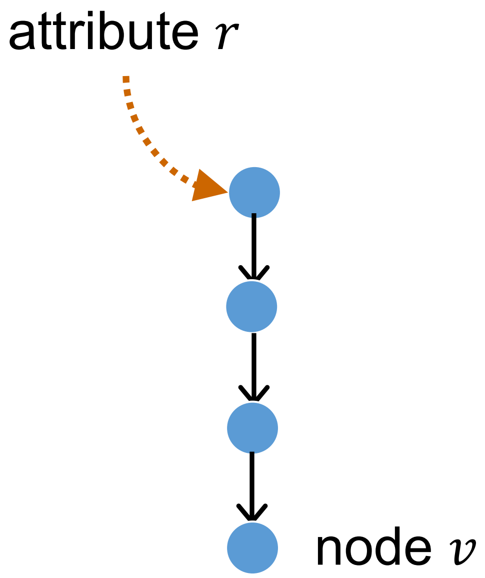


Two Types of Random Walks







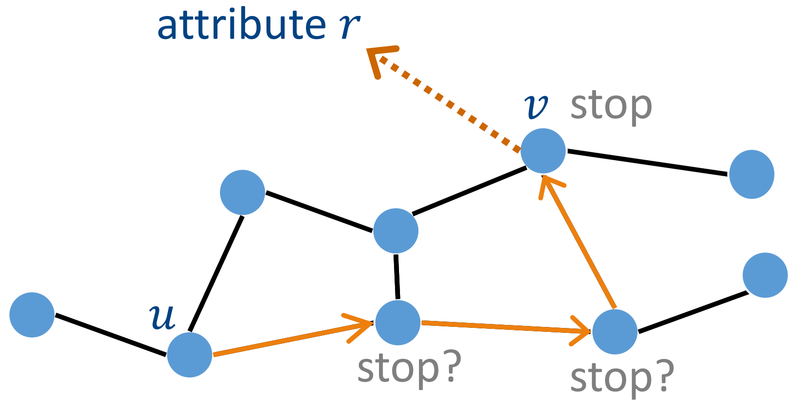


Forward: node-to-attribute

Backward: attribute-to-node

Forward Random Walks

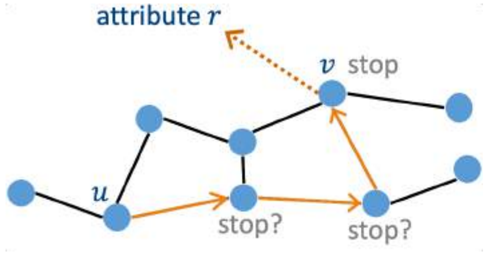
- Forward random walk from node u:
  - Start from u
  - At each step, stop with α probability
  - After stopping at a node v, pick an attribute r with probability $\propto \mathrm{w}(v, r)$
- Intuition: it samples an attribute r from the vicinity of u
- $p_f(u, r)$ is the probability that a forward random walk from u samples r in the end



Node-Attribute Affinity

- Our node-attribute affinity measure:

$$\mathbf{F}[u,r] = \log\left(\frac{|V| \cdot p_f(u,r)}{\sum_{v\in V} p_f(v,r)} + 1\right)$$

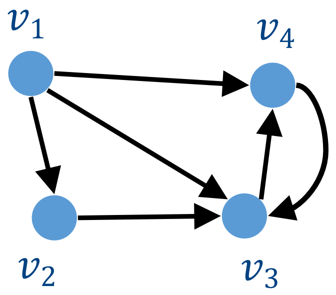


- Understand $\mathbf{F}[u,r]$ using PMI (pointwise mutual information) in information theory:
  - PMI $\log(\frac{\Pr(r|v)}{\Pr(r)})$ measures the co-occurrence of elements and in a collection of elements S
  - all random walks as S, $\sum_{v\in V} p_f(v,r)$ as $\Pr(r)$ and $p_f(u,r)$ as $\Pr(r|v)$
  - $\mathbf{F}[u,r]$ measures how frequently u, r co-occur on all random walks to r
  - Word2vec is implicitly factorizing a PMI matrix to obtain word embeddings [Levy NeurIPS'14]

Levy et al. Neural word embedding as implicit matrix factorization. NeurIPS 2014.

Computing $\mathbf{F}$

- Node-attribute affinity
  - $\mathbf{F}[u,r] = \log\left(\frac{|V|\cdot p_f(u,r)}{\sum_{v\in V} p_f(v,r)} + 1\right)$
  - $p_f(u,r) = \alpha \sum_{i=0}^{t} (1-\alpha)^i \mathbf{P}^i \cdot \mathbf{R}_r[u,r]$
  - $O(mdt)$ time using power method

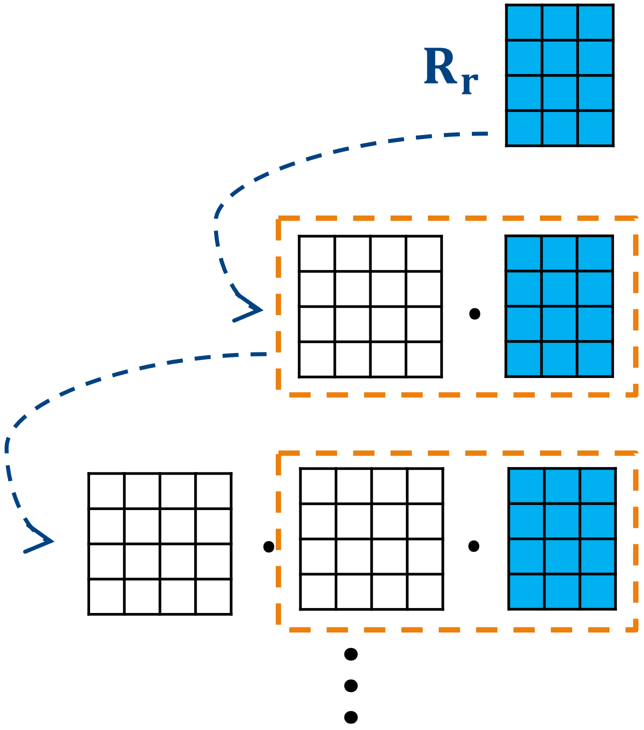


$$\begin{array}{c|cccc} & v_1 & v_2 & v_3 & v_4 \\ \hline v_1 & 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ v_2 & 0 & 0 & 1 & 0 \\ v_3 & 0 & 0 & 0 & 1 \\ v_4 & 0 & 0 & 1 & 0 \end{array}$$

Transition matrix $\mathbf{P}$

$$\begin{array}{c|ccc} & r_1 & r_2 & r_3 \\ \hline v_1 & 1/2 & 1/2 & 0 \\ v_2 & 1/3 & 0 & 2/3 \\ v_3 & 1/3 & 1/3 & 1/3 \\ v_4 & 1 & 0 & 0 \end{array}$$

Row-normalized attribute matrix $\mathbf{R}_r$



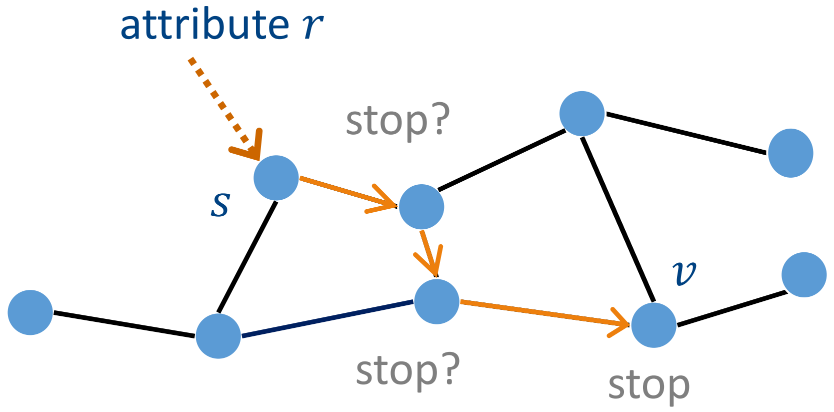
Weighted sum

Backward RW & Attribute-Node Affinity

- Backward random walk from attribute r
  - Randomly pick a node s with probability $\propto \mathrm{w}(s, r)$
  - Start a random walk from s
  - At each step, stop with α probability
  - Let v be the stopping point of the walk
- Our attribute-to-node affinity measure:

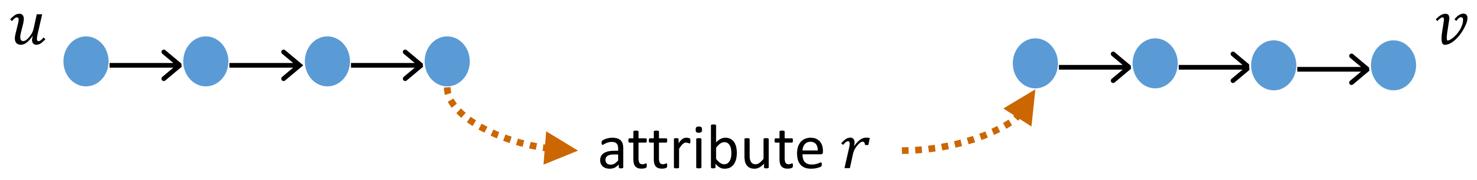
$$\mathbf{B}[r, v] = \log\left(\frac{|R| \cdot p_b(r, v)}{\sum_{r' \in R} p_b(r', v)} + 1\right)$$

  - where R is the set of all attributes,
  - $p_b(r, v)$ is the probability that a backward random walk from r samples v in the end



Why node-attribute & attribute-node affinities

- We can indirectly model node-node affinities with much less space using node-attribute + attribute-node affinities

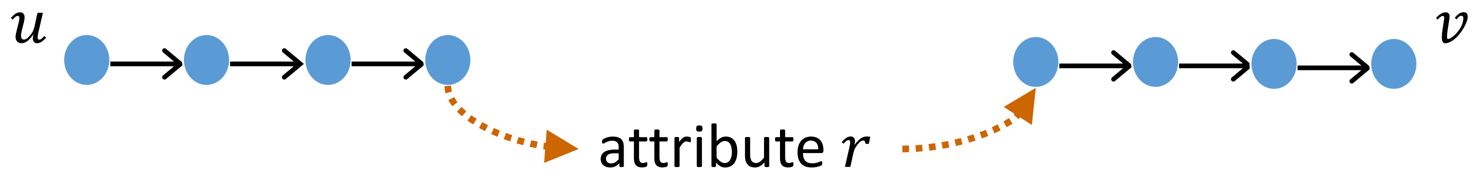


- Intuition:
  - Consider a forward random walk from u to r & a backward random walk from r to v
  - They form an extended walk from u to v, in which we "teleport" through a virtual connection by r
  - Such random walks could be combined to model node-node affinity

Capturing node-node affinity

- Our node-node affinity can be indirectly constructed via:

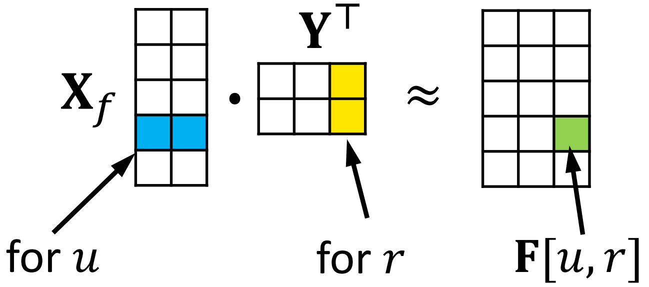
$$p(u, v) = \sum_{r \in R} \mathbf{F}[u, r] \cdot \mathbf{B}[r, v]$$

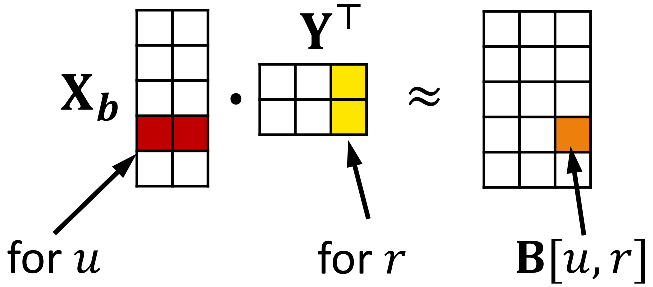


- Thus, we do not need an $n \times n$ node-node affinity matrix explicitly
  - space overhead: $O(n^2) \rightarrow O(nd), d \ll n$
  - d = #attributes, n = #nodes

Objective function

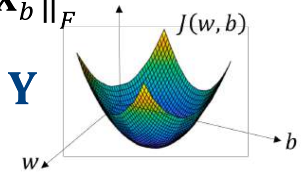
- We construct
  - two embedding matrices $\mathbf{X}_f, \mathbf{X}_b \in \mathbb{R}^{n\times k}$ for the nodes, and
  - one embedding matrix $\mathbf{Y} \in \mathbb{R}^{d\times k}$ for attributes
- Optimization objective:
  - $\min_{\mathbf{X}_f,\mathbf{Y},\mathbf{X}_b} \left\|\mathbf{F} - \mathbf{X}_f\mathbf{Y}^\top\right\|_F^2 + \left\|\mathbf{B} - \mathbf{X}_b\mathbf{Y}^\top\right\|_F^2$
  - $\mathbf{X}_f \cdot \mathbf{Y}^\top \approx \mathbf{F}$, to capture node-attribute affinity
  - $\mathbf{X}_b\mathbf{Y}^\top \approx \mathbf{B}$, to capture attribute-node affinity



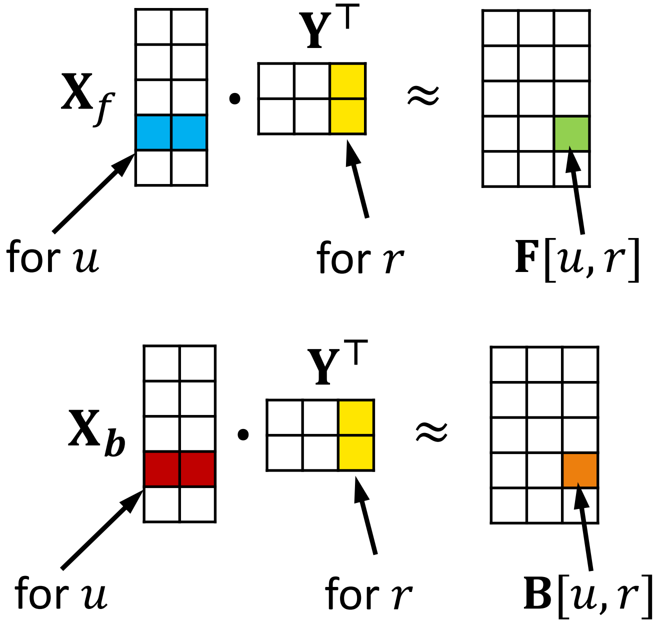


Solving the optimization objective

- Optimization objective:
  - $\min_{\mathbf{X}_f, \mathbf{Y}, \mathbf{X}_b} \left\| \mathbf{F} - \mathbf{X}_f \mathbf{Y}^{\mathsf{T}} \right\|_F^2 + \left\| \mathbf{B} - \mathbf{Y} \cdot \mathbf{X}_b^{\mathsf{T}} \right\|_F^2$
- We can obtain $\mathbf{X}_f$, $\mathbf{X}_b$, and $\mathbf{Y}$ using gradient descent



  - a large number of iterations are required till convergence
  - jointly updating $\mathbf{X}_f$, $\mathbf{X}_b$ and $\mathbf{Y}$ involves intensive computation
- Our idea for efficiency:
  - find a good initialization for $\mathbf{X}_f$, $\mathbf{X}_b$ and $\mathbf{Y}$ based on singular value decomposition (SVD)

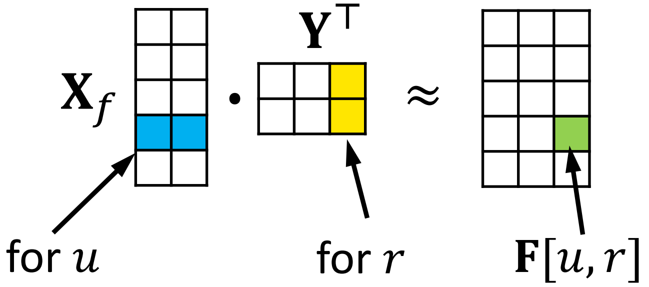


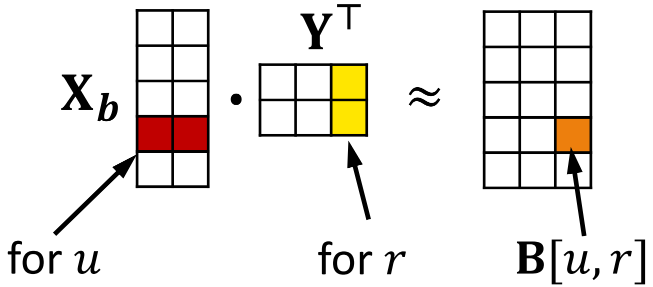
Initialize embeddings via SVD

- Initial solution for the first part via randomized SVD

$$\mathbf{F} \approx \underbrace{\boxed{\mathbf{U} \cdot \mathbf{\Sigma}}}_{\mathbf{X}_f} \cdot \underbrace{\boxed{\mathbf{V}}}_{\mathbf{Y}}^{\mathrm{T}}$$

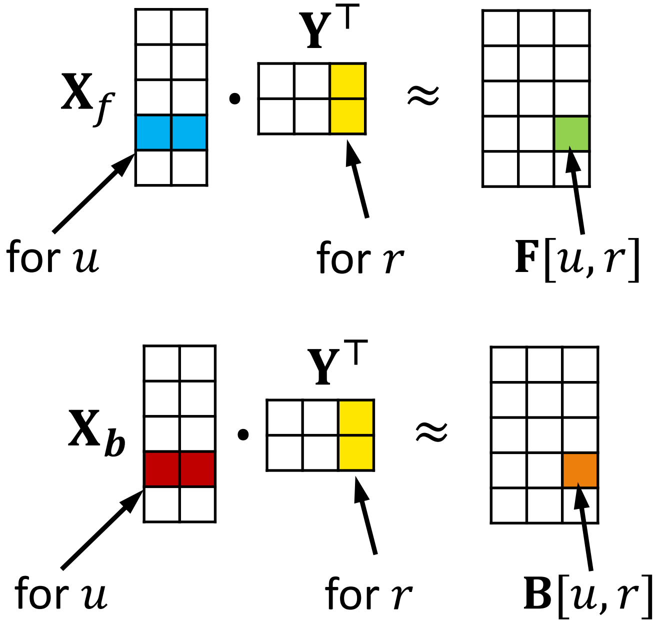
- Initial solution for the second part
  - approximate singular vectors $\mathbf{Y}$=$\mathbf{V}$ is semi-unitary, i.e., $\mathbf{Y}^{\mathrm{T}}\mathbf{Y} = \mathbf{I}$
  - Intuitively, if we want $\mathbf{X}_b\mathbf{Y}^{\mathrm{T}} = \mathbf{B}$, $\mathbf{X}_b = \boxed{\mathbf{X}_b\mathbf{Y}^{\mathrm{T}}}\mathbf{Y} = \boxed{\mathbf{B}} \cdot \mathbf{Y}$



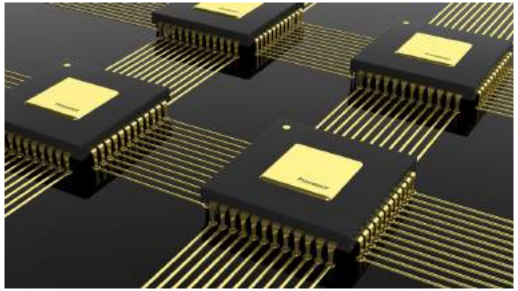


Space & time complexities

- Time complexity:
  - $O(mdt + ndkt)$
  - t = #iterations of gradient descent ($t = 5$ in our experiments)
  - k = the embedding size
  - m = #edges
  - n = #nodes
  - d = #attributes
- Space complexity
  - $O(m + nd + nk)$



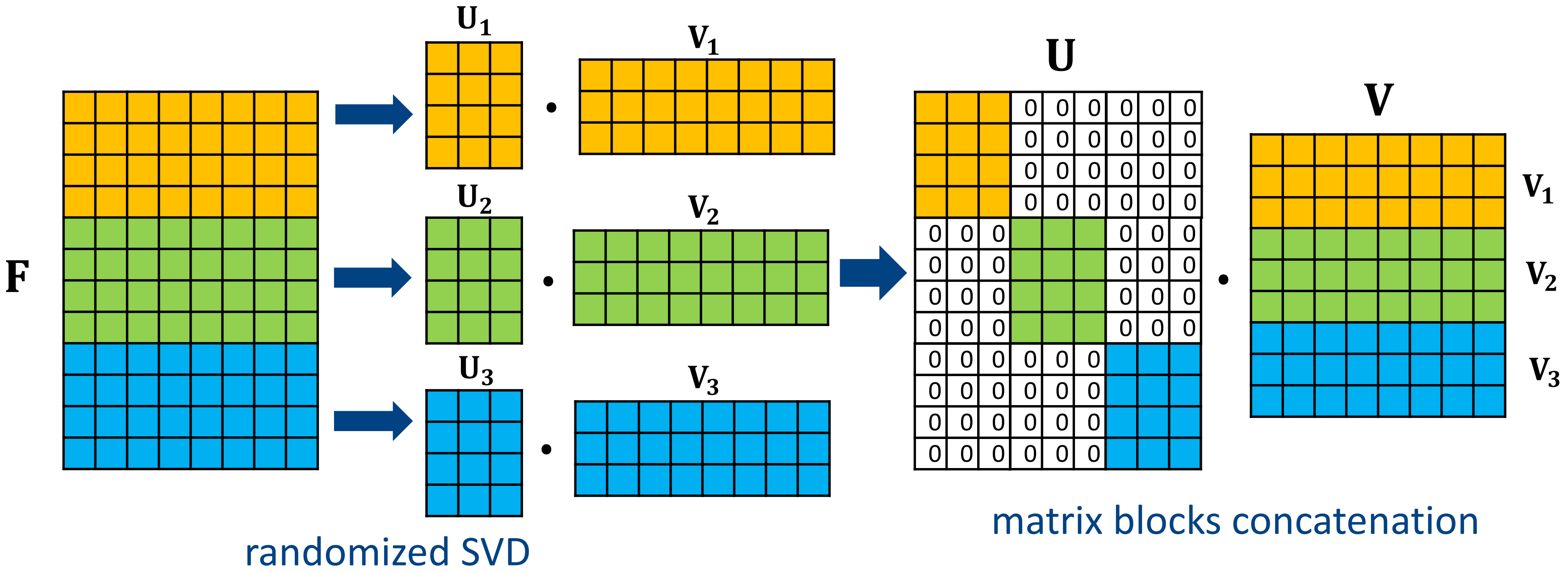
Parallel implementation of PANE



- Parallel computation of $\mathbf{F}$ and $\mathbf{B}$
  - Matrix multiplications can be easily parallelized
- Parallel gradient descent. In each iteration,
  - $\mathbf{X}_f[u]\ \forall u \in V$ or $\mathbf{X}_b[v]\ \forall v \in V$ can be updated independently
  - $\mathbf{Y}[r]$ for each attribute r can be updated independently
- Parallel SVD over $\mathbf{F}$
  - The SVD over $\mathbf{F} \neq$ direct SVD over each matrix blocks of $\mathbf{F}$
  - How to perform SVD over $\mathbf{F}$ in parallel?

Parallel SVD

- Given $\mathbf{F} \in \mathbb{R}^{12\times 8}$, we want $\mathbf{X}_f \in \mathbb{R}^{12\times 3}$ and $\mathbf{Y} \in \mathbb{R}^{8\times 3}$ s.t. $\mathbf{X}_f \cdot \mathbf{Y}^\top \approx \mathbf{F}$



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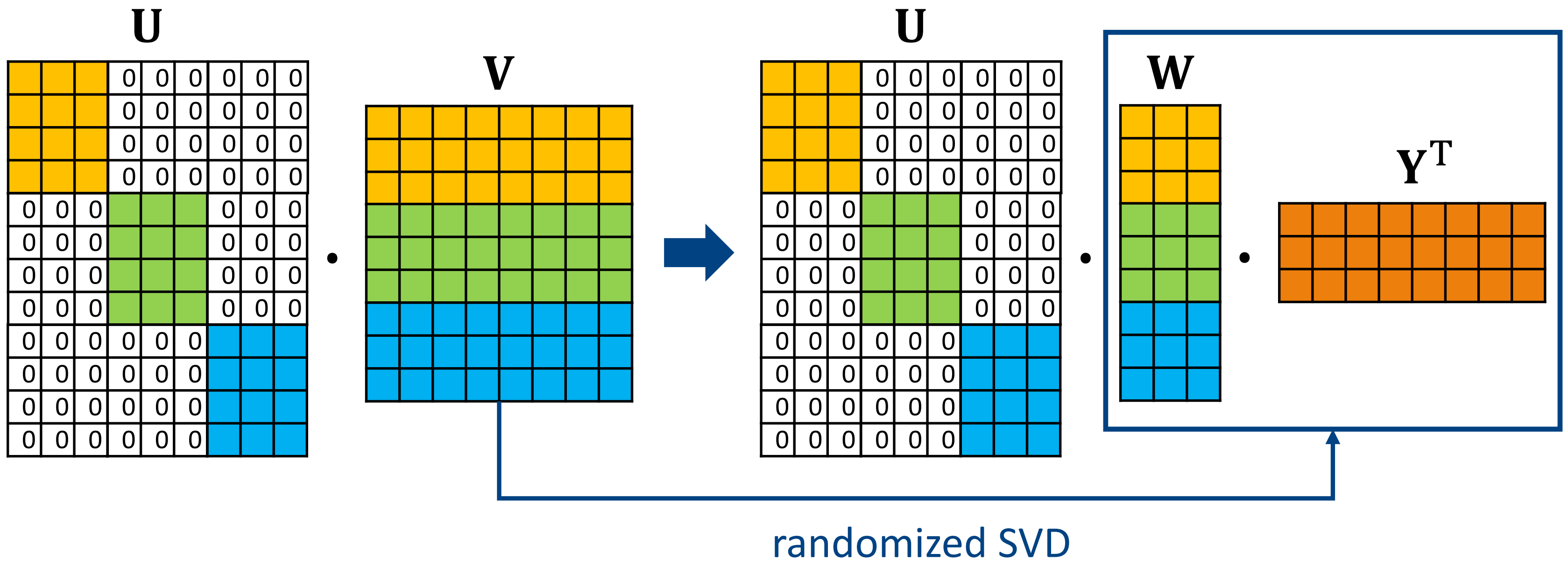

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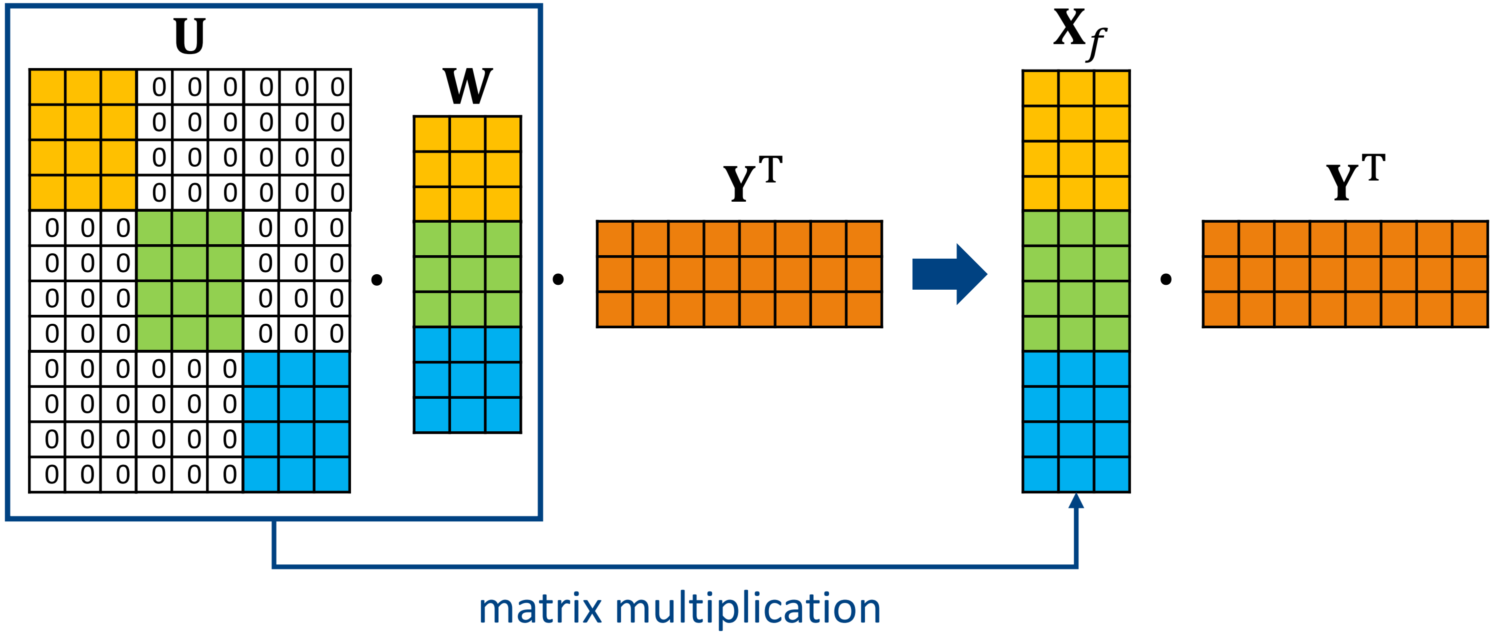

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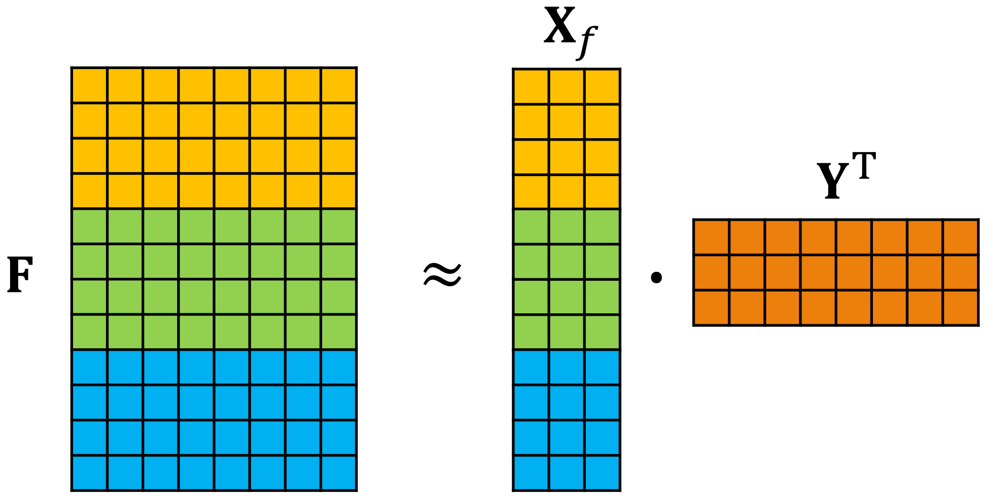


Experiments: Datasets

Name	# of nodes	# of edges	# of distinct attributes	# of attributes per node	# of distinct labels
Cora	2.7k	5.4k	1.4k	18.2	7
Citeseer	3.3k	4.7k	3.7k	31.9	6
Facebook	4k	88.2k	1.3k	8.3	193
Pubmed	19.7k	44.3k	0.5k	50.2	3
Flickr	7.6k	479.5k	12.1k	24.0	9
Google+	107.6k	13.7M	15.9k	2793.7	468
TWeibo	2.3M	50.7M	1.7k	7.3	8
MAG	59.3M	978.2M	2.0k	7.3	100

Experiments: Competitors

- PANE: Our solution for attributed graphs
- Default embedding dimensionality: $k = 128$
- CPU: Intel Xeon 2.2GHz

- 6 neural-based methods

STNE	[KDD 2018]
ARGA	[IJCAI 2018]
LQANR	[IJCAI 2019]
CAN	[WSDM 2019]
DGI	[ICLR 2019]
GATNE	[KDD 2019]

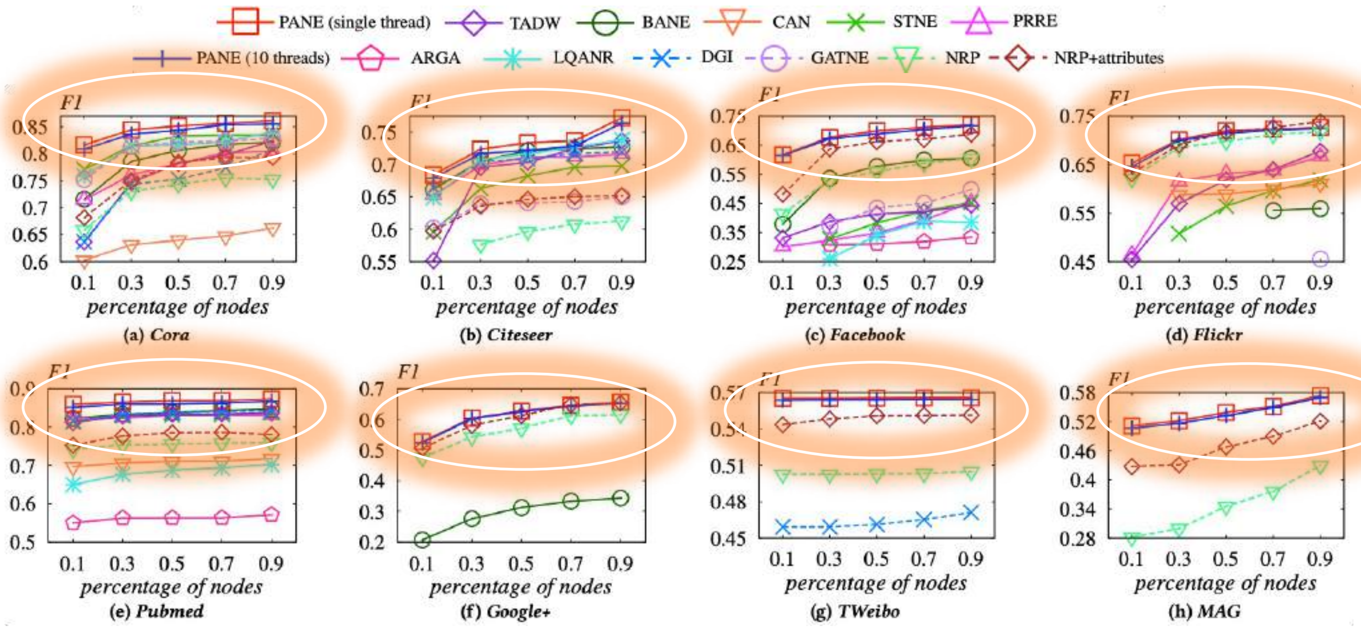
- 3 factorization-based methods

TADW	[IJCAI 2015]
BANE	[ICDM 2018]
NRP	[VLDB 2020]

- 1 other method

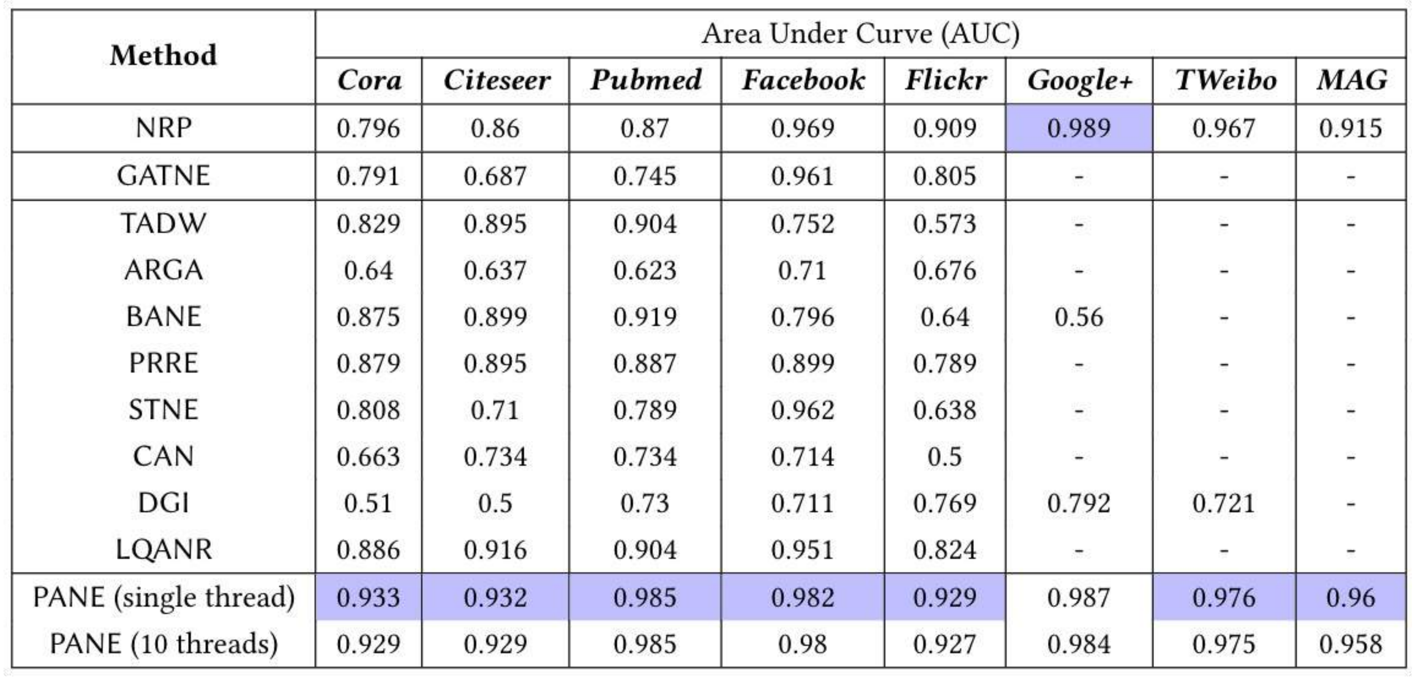
PRRE	[CIKM 2018]

Results: Node Classification



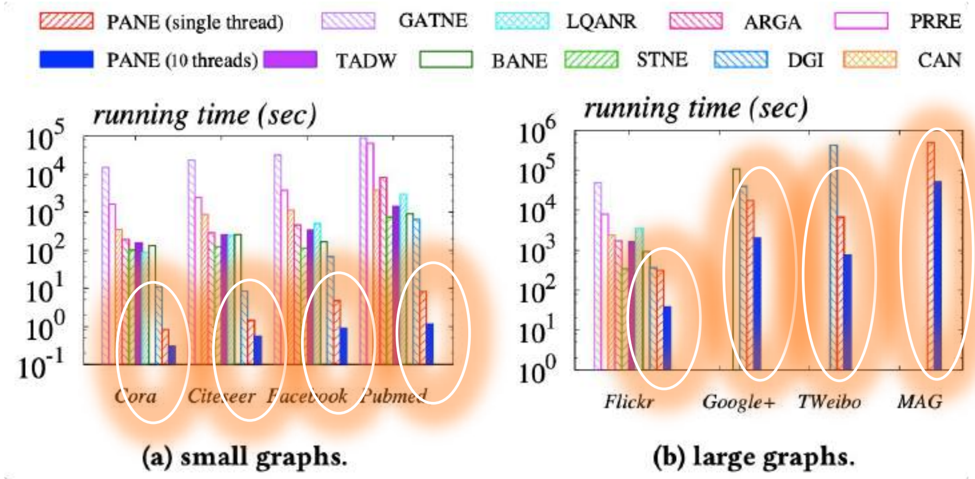
- Percentage of nodes used for training: 10% ~ 90%
- PANE vs. SOTA: improvements of 3.4%-17.2% in terms of F1 measure

Results: Link Prediction



Method	Area Under Curve (AUC)							
	Cora	***Citeseer***	***Pubmed***	***Facebook***	***Flickr***	***Google+***	***TWeibo***	***MAG***
NRP	0.796	0.86	0.87	0.969	0.909	0.989	0.967	0.915
GATNE	0.791	0.687	0.745	0.961	0.805	-	-	-
TADW	0.829	0.895	0.904	0.752	0.573	-	-	-
ARGA	0.64	0.637	0.623	0.71	0.676	-	-	-
BANE	0.875	0.899	0.919	0.796	0.64	0.56	-	-
PRRE	0.879	0.895	0.887	0.899	0.789	-	-	-
STNE	0.808	0.71	0.789	0.962	0.638	-	-	-
CAN	0.663	0.734	0.734	0.714	0.5	-	-	-
DGI	0.51	0.5	0.73	0.711	0.769	0.792	0.721	-
LQANR	0.886	0.916	0.904	0.951	0.824	-	-	-
PANE (single thread)	0.933	0.932	0.985	0.982	0.929	0.987	0.976	0.96
PANE (10 threads)	0.929	0.929	0.985	0.98	0.927	0.984	0.975	0.958

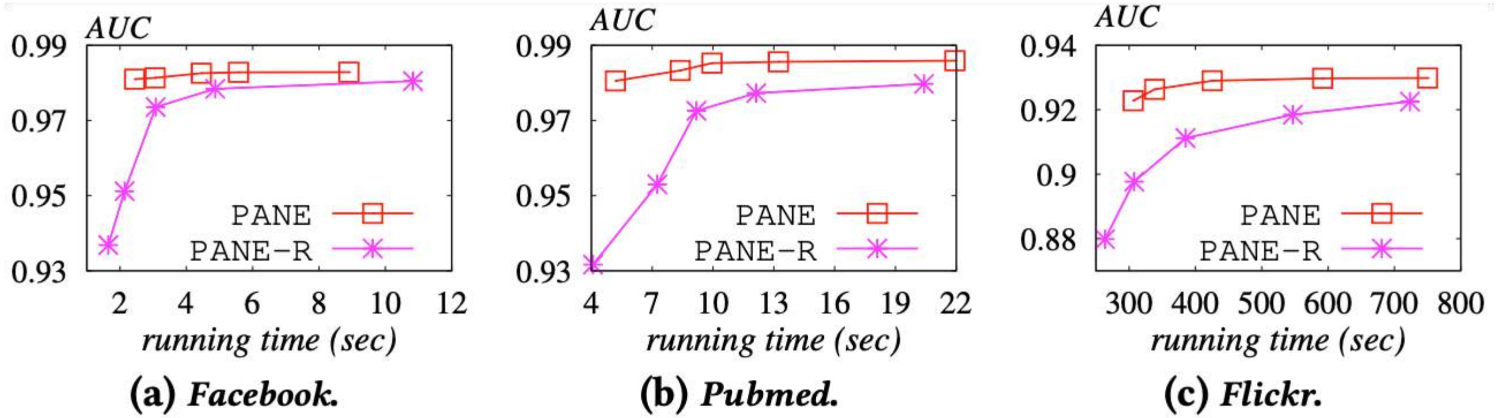
Results: Efficiency



- Compared to the state of the art, PANE is orders of magnitude faster
- On the MAG dataset with 0.98 billion edges, PANE can terminate within 12 hours using 10 CPU cores (Intel Xeon 2.2GHz)

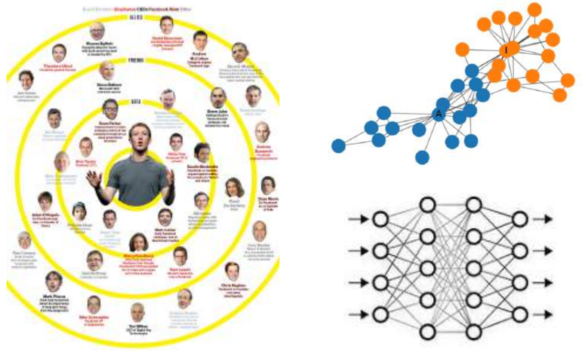
Effectiveness of SVD-based initializations

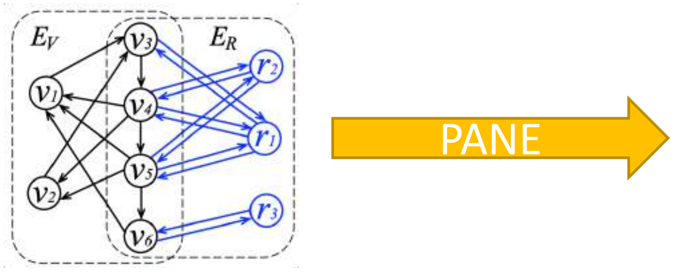
PANE-R: the algorithm that uses random initializations
PANE: the algorithm that uses SVD-based initializations

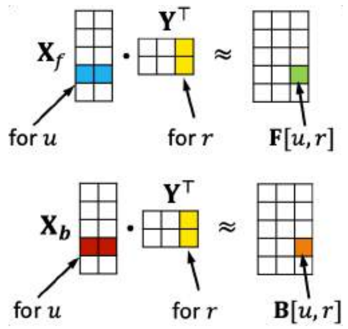


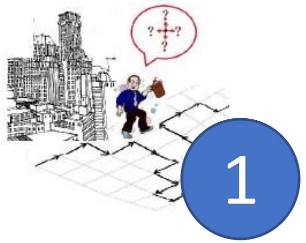
Link prediction performance vs. running time
when varying #iteration for the gradient descent from 1 to 20

THANK YOU

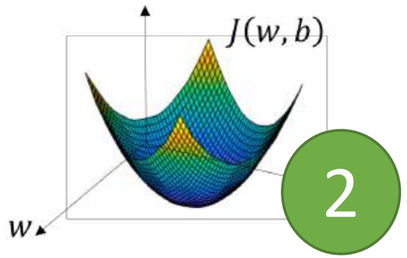




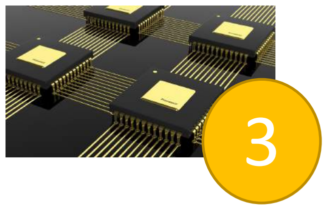




Random walks



Joint matrix factorization



Parallelization