



Optimization Techniques for Structural Similarity Computation on Large Networks

Presented by

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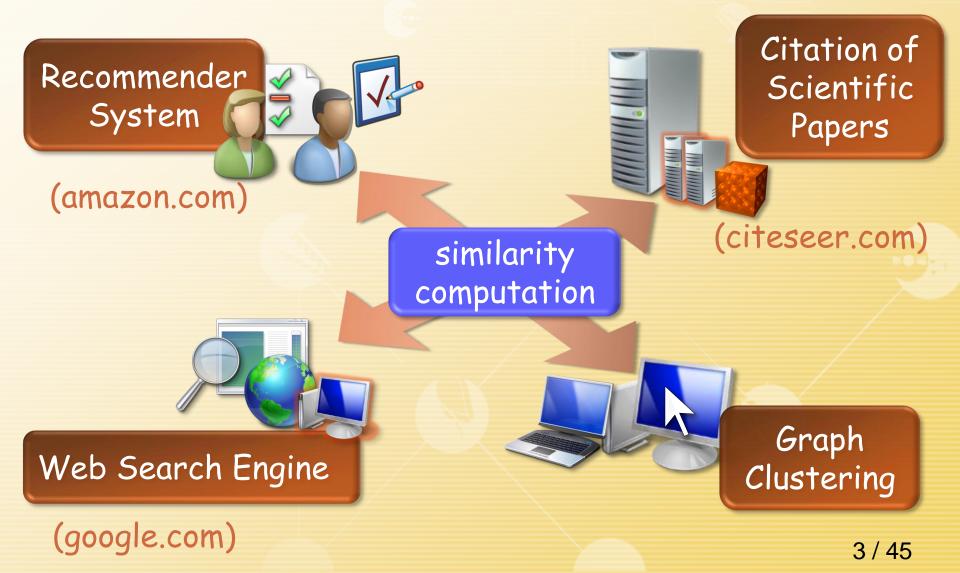






1 Background

Many applications require a measure of similarity between objects.





1 Background

Text-based Similarity (content)

• Cosine similarity $\sigma_{\text{cosine}} = \frac{|\Gamma_i \cap \Gamma_j|}{\sqrt{|\Gamma_i||\Gamma_j|}}$ Jaccard index $\sigma_{\text{Jaccard}} = \frac{|\Gamma_i \cap \Gamma_j|}{|\Gamma_i \cup \Gamma_j|}$

Link-based Similarity (structure)

- PageRank [Larry Page, Google Tech. Rep.' 99]
 - One page's authority is decided by its neighbors' authorities.
- SimRank [Jeh and Widom, SIGKDD'02]
- Penetrating-Rank [Zhao et. al, CIKM'09]
 - Two objects are similar if they are referenced by similar objects.
- SimFusion [Xi et. al, SIGIR'05]
 - The similarity between two data objects is reinforced by the similarity of their related objects.



1 Background

The success of Google PageRank has demystified the importance of link-based similarity measure.

A space and time efficient algorithm for SimRank computation dl.acm.org/citation.cfm?id=2158804 - 翻译此页 作者:WYu - 2012 - 被引用次数:6 - 相关文章

A space and time efficient algorithm for SimRank computation, 2012 Article. Bibliometrics Data Bibliometrics. · Downloads (6 Weeks): n/a · Downloads (12 ...

- Merits of link-based similarity measure:
 - Applicable to any domain with object-to-object relationships (It is a graph-theoretic model that reflects a better human intuition with a solid rationale.)
 - No requirement of extra human-built hierarchies (It purely hinges on the structure of linkage patterns.)
 - Possessing good expansibility

(It can be combined with other domain-specific measures.)



2 Aims and Objectives

- Huge networks have been mounting up, calling for new techniques to efficiently handle similarity computations on large-scale graphs.
 - the increasing scale of the Web
 - the ubiquity of the Internet

- High CPU time !! High RAM space !!
- My research topic aims to develop, analyze, implement and evaluate novel approaches to optimize link-based similarity computation.
 - speed up the computations of the existing similarity models (i.e., SimRank, SimFusion, P-Rank)
 - improve existing models for effectively measuring similarity
 - develop a user-friendly system prototype for evaluation



3 Challenges

Focus on optimizing SimRank, SimFusion, P-Rank:

- To reduce the complexity of the best-known algorithms
 - computational time
 - memory space
 - convergence rate
- To accurately compute the similarity scores
 - accuracy estimate
 - stability & sensitivity analysis
- To extend the existing models
 - ♦ static graphs → dynamic networks
 - \diamond single machine \rightarrow parallel version

efficiency

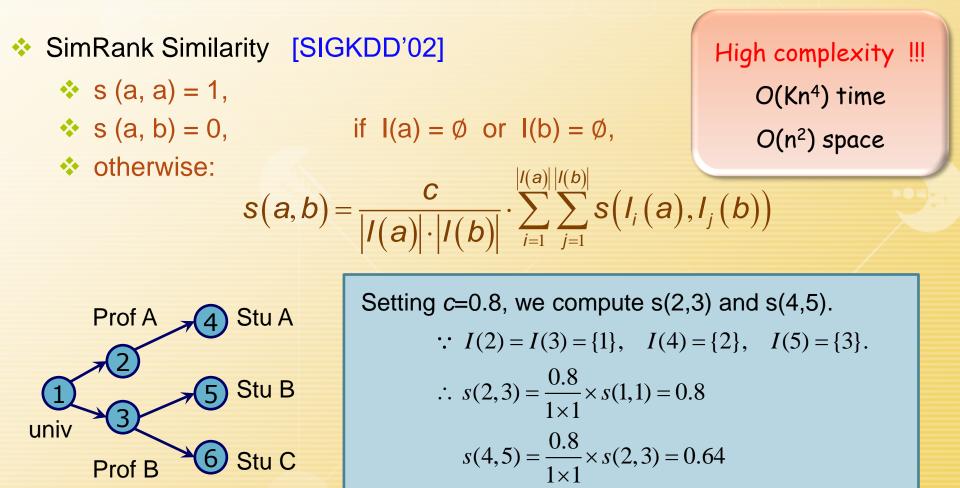
scalability

effectiveness



SimRank Measure

♦ Given a network G=(V,E), and a link-based scoring function s: V x V → [0,1], it is to efficiently compute similarity scores of all vertex-pairs in G.





4 State of the Arts : Related Work

Deterministic Method [SIGKDD'02, VLDBJ'10]

(following the fixed-point iteration to compute similarity)

$$\mathbf{s}^{(k+1)}(a,b) = \frac{c}{|I(a)| \cdot |I(b)|} \cdot \sum_{i=1}^{|I(a)|} \sum_{j=1}^{|I(a)|} \mathbf{s}^{(k)}(I_i(a), I_j(b))$$

- ✓ Advantage: accuracy guarantee
- Disadvantage: high time and space (cubic time and quadratic space)
- Probabilistic Method [EDBT'05, TKDE'05]

(utilizing the Monte-Carlo sampling approach to estimate similarity)

 $S(a,b) = E(c^{\tau(a,b)})$

✓ Advantage: scalability on large graphs (linear time and space)
 ✓ Disadvantage: low estimation quality



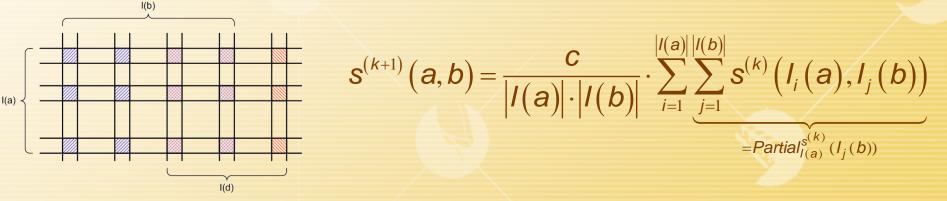
4 State of the Arts : Related Work

[Lizorkin et al., VLDB J.'10]

- Main Contributions.
 - A precise accuracy estimate is presented for SimRank iteration.

 $\left|s^{(k)}(a,b)-s(a,b)\right|\leq c^{k+1}$

A partial sum function is utilized to improve SimRank computational complexity from O(kn⁴) to O(kn³).



A threshold sieving heuristic is introduced and its accuracy estimation is given that further improves the efficiency.



5.1 Contributions: SimRank

Motivation:

The high complexity of time and space is still a mighty obstacle in using SimRank on large networks.

Paper	Computational Time	Space	Accuracy
SIGKDD '02	$\mathcal{O}\left(Kn^4 ight)$	$\mathcal{O}\left(n^2 ight)$	not given
VLDB J. '10	$\mathcal{O}\left(Kn^3\right)$	$\mathcal{O}\left(n^2 ight)$	c^{K}
EDBT '10	$O((r^3+1)rn^2+r^4)$	$\mathcal{O}\left(r^2n^2+r^4\right)$	not given
future work	$\mathcal{O}\left(rm + r^2n + Kr^3\right)$	$\mathcal{O}\left(rn ight)$	$c^{2^K} + \frac{1}{\sqrt{n}}$

- SimRank computation is iterative in nature, but no prior work has studied the stability of SimRank, which can
 - (i) gauge the sensitivity of similarity to the perturbations in the link structure (e.g., by adding or removing edges)
 - (ii) imply whether large amounts of accumulated round-off errors will run the risk of producing nonsensical similarity.



5.1 Contributions: SimRank

Main Contributions: **

••• A "squaring memoization" technique is devised for SimRank convergence computation, which cuts down the number of iterations exponentially for a given accuracy.

time / space complexity

*

•••

rate

An order-r (\ll n) Krylov subspace is deployed for speeding up SimRank computation in $\mathcal{O}(rm + r^2n + K'r^3)$ time and $\mathcal{O}(rn)$ space up to an additive error of $\left(c^{2^{K'}} + \frac{1}{\sqrt{n}}\right)$ for any vertex-pair.

stability

A notion of SimRank condition number is introduced, and a tight bound of this number is provided, aiming at analyzing similarity stability.



1) Speed up Convergence Rate

Naïve SimRank Iterative Paradigm.

[Lizorkin et al., VLDB J.'10]

$$\begin{cases} \mathbf{S}^{(0)} = (1-c) \cdot \mathbf{I}_n, \\ \mathbf{S}^{(k+1)} = c \cdot \mathbf{Q} \cdot \mathbf{S}^{(k)} \cdot \mathbf{Q}^T + (1-c) \cdot \mathbf{I}_n. \end{cases}$$

 $\|\mathbf{S}^{(k)} - \mathbf{S}\|_{\max} \le c^{k+1}$

Squaring Memoization" Paradigm.

$$\begin{cases} \mathbf{S}_{\langle 2 \rangle}^{(0)} = (1-c) \cdot \mathbf{I}_n, \\ \mathbf{S}_{\langle 2 \rangle}^{(k+1)} = \mathbf{S}_{\langle 2 \rangle}^{(k)} + c^{2^k} \cdot \mathbf{Q}^{2^k} \cdot \mathbf{S}_{\langle 2 \rangle}^{(k)} \cdot \left(\mathbf{Q}^{2^k}\right)^T \qquad \|\mathbf{S}_{\langle 2 \rangle}^{(k)} - \mathbf{S}\|_{\max} \le c^{2^k} \end{cases}$$

Main Idea:

• Once squared, the matrix \mathbf{Q}^{2^k} is memoized for the next iteration and thus will not be recomputed when subsequently needed.

$$\mathbf{Q}^{2^k} = \underbrace{\mathbf{Q} \cdot \mathbf{Q} \cdots \mathbf{Q}}_{2^k}$$

$$\mathbf{Q}^{2^{k}} = \underbrace{\left(\left(\left(\mathbf{Q}^{2}\right)^{2}\right)^{2}\cdots\right)^{2}}_{k}$$



1) Speed up Convergence Rate

Naïve SimRank Iterative Paradigm"Squaring Memoization" Paradigm $\mathbf{S}^{(0)} = (1-c) \cdot \mathbf{I}_n$ $\mathbf{S}^{(0)}_{(2)} = (1-c) \cdot \mathbf{I}_n$ $\mathbf{S}^{(1)} = (1-c) \cdot \left[\mathbf{I}_n + c\mathbf{Q}\mathbf{Q}^T + c^2\mathbf{Q}^2(\mathbf{Q}^2)^T\right]$ $\mathbf{S}^{(2)}_{(2)} = (1-c) \cdot \left[\mathbf{I}_n + c\mathbf{Q}\mathbf{Q}^T + c^2\mathbf{Q}^2(\mathbf{Q}^2)^T + c^3\mathbf{Q}^3(\mathbf{Q}^3)^T\right]$ $\mathbf{S}^{(2)} = (1-c) \cdot \left[\mathbf{I}_n + c\mathbf{Q}\mathbf{Q}^T + c^2\mathbf{Q}^2(\mathbf{Q}^2)^T + c^3\mathbf{Q}^3(\mathbf{Q}^3)^T\right]$ $\mathbf{S}^{(2)}_{(2)} = (1-c) \cdot \left[\mathbf{I}_n + c\mathbf{Q}\mathbf{Q}^T + c^2\mathbf{Q}^2(\mathbf{Q}^2)^T + c^3\mathbf{Q}^3(\mathbf{Q}^3)^T\right]$ $\mathbf{S}^{(7)} = (1-c) \cdot \sum_{i=0}^{7} c^i \mathbf{Q}^i(\mathbf{Q}^i)^T$ $\mathbf{S}^{(3)}_{(2)} = (1-c) \cdot \sum_{i=0}^{7} c^i \mathbf{Q}^i(\mathbf{Q}^i)^T$

$$\mathbf{S}_{\langle 2\rangle}^{(k)} = \mathbf{S}^{(2^k - 1)}$$

 In each step of "squaring memoization" iteration, one actually computes exponential steps (with base 2) of the conventional iteration. As a result, the convergence rate of "squaring memoization" iteration becomes exponentially faster than that of conventional iteration.



1) Speed up Convergence Rate

Squaring Memoization" Paradigm.

$$\begin{cases} \mathbf{S}_{\langle 2 \rangle}^{(0)} = (1-c) \cdot \mathbf{I}_n, \\ \mathbf{S}_{\langle 2 \rangle}^{(k+1)} = \mathbf{S}_{\langle 2 \rangle}^{(k)} + c^{2^k} \cdot \mathbf{Q}^{2^k} \cdot \mathbf{S}_{\langle 2 \rangle}^{(k)} \cdot \left(\mathbf{Q}^{2^k}\right)^T \qquad \qquad \|\mathbf{S}_{\langle 2 \rangle}^{(k)} - \mathbf{S}\|_{\max} \le c^{2^k} \end{cases}$$

Extending to the "u-th Powering Memoization" Paradigm: (u=2, 3,...)

$$\begin{cases} \mathbf{S}_{\langle u \rangle}^{(0)} = (1-c) \cdot \mathbf{I}_{n}, \\ \mathbf{S}_{\langle u \rangle}^{(k+1)} = \sum_{i=0}^{u-1} c^{i \cdot u^{k}} \cdot \mathbf{Q}^{i \cdot u^{k}} \cdot \mathbf{S}_{\langle u \rangle}^{(k)} \cdot (\mathbf{Q}^{i \cdot u^{k}})^{T}, \qquad \left\| \mathbf{S}_{\langle u \rangle}^{(k)} - \mathbf{S} \right\|_{\max} \leq c^{u^{k}} \end{cases}$$

Complexity:

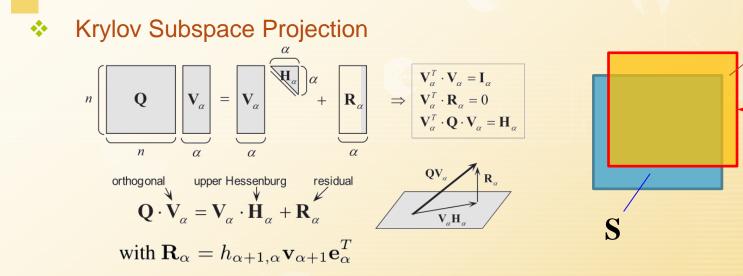
FLOPs per iteration#-iterationstotalnaïve $O(n^3)$ $\lceil \log_c \epsilon \rceil - 1$ $O((\lceil \log_c \epsilon \rceil - 1) n^3)$ u-th Powering $O((u-1) \cdot n^3)$ $\lceil \log_u \log_c \epsilon \rceil$ $O(\lceil \log_u \log_c \epsilon \rceil (u-1) n^3)$

Squaring Memoization" achieves the best computational performance.

$$\mathcal{O}(f(u))$$
 with $f(u) = \left\lceil \ln(\log_c \epsilon) \right\rceil \cdot \frac{u-1}{\ln u} \cdot n^3$ $(u = 2, 3, \cdots)$



2) Improve Computational Efficiency



Main Idea

- A projection of the matrix Q (n x n dimension) onto a Krylov subspace (α x α dimension with α ≪ n) is used for computing similarity.
- Due to its smaller dimension, the Krylov subspace based SimRank formula is relatively easier to solve with accuracy guarantees.

Krylov subspace ($\alpha \times \alpha$) $\mathbf{S}_{\alpha} = c \cdot \mathbf{H}_{\alpha} \cdot \mathbf{S}_{\alpha} \cdot \mathbf{H}_{\alpha}^{T} + (1 - c) \cdot \mathbf{I}_{\alpha}$ \downarrow $\hat{\mathbf{S}}_{\alpha} = \mathbf{V}_{\alpha} \cdot \mathbf{S}_{\alpha} \cdot \mathbf{V}_{\alpha}^{T}$ original space (n x n)

 $\hat{\mathbf{S}}_{\alpha}$

 $\mathbf{S} = c \cdot (\mathbf{Q} \cdot \mathbf{S} \cdot \mathbf{Q}^T) + (1 - c) \cdot \mathbf{I}_n$



2) Improve Computational Efficiency

Error Estimate

LEMMA. Let Err(*) be a matrix function defined by

$$Err(\mathbf{X}) \stackrel{def}{=} c \cdot \mathbf{Q} \cdot \mathbf{X} \cdot \mathbf{Q}^{T} - \mathbf{X} + (1 - c) \cdot \mathbf{I}_{n}, \quad (\mathbf{X} \in \mathbb{R}^{n \times n})$$

Then for every $\alpha = 1, 2, \dots, n$, we have

$$\|Err(\hat{\mathbf{S}}_{\alpha})\|_{2} \leq \epsilon_{\alpha},$$

where

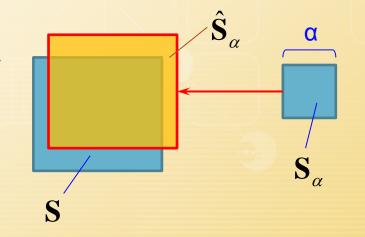
$$\epsilon_{\alpha} = 1 - c \left(1 - h_{\alpha+1,\alpha} \sqrt{2 \| \mathbf{H}_{\alpha} [\mathbf{S}_{\alpha}]_{\star,\alpha} \|_{2}^{2} + h_{\alpha+1,\alpha}^{2} [\mathbf{S}_{\alpha}]_{\alpha,\alpha}^{2}} \right)$$

COROLLARY 1. $\|\operatorname{Err}(\hat{\mathbf{S}}_r)\|_2 \leq 1 - c.$

THEOREM. For every $\alpha = 1, 2, \dots, n$, the following estimate holds:

$$\|\mathbf{S} - \mathbf{\hat{S}}_{\alpha}\|_{2} \leq \frac{\sqrt{n}}{1-c} \cdot \|Err(\mathbf{\hat{S}}_{\alpha})\|_{2}$$

COROLLARY 2. $\|\mathbf{S} - \hat{\mathbf{S}}_r\|_2 \leq \sqrt{n}.$





3) The Complete Framework

Integrated with "Squaring Memoization".

Error Estimate.

$$\|\mathbf{S} - \hat{\mathbf{S}}_{\alpha}^{(k)}\|_{2} \leq \epsilon, \text{ with } \epsilon = n \cdot c^{2^{k}} + \frac{\sqrt{n}}{1-c} \cdot \epsilon_{c}$$

COROLLARY 3.

$$\frac{1}{n}\sqrt{\sum_{i,j=1}^{n} \left([\mathbf{S}]_{i,j} - [\hat{\mathbf{S}}_{r}^{(k)}]_{i,j} \right)^{2}} \le c^{2^{k}} + \frac{1}{\sqrt{n}}$$

Complexity Analysis.

Operation	Time	Space	Error
building Krylov subspace	0 (rm)	0 (rn)	
computing $\mathbf{S}_r^{(K)}$ in the subspace	O(Kr ³)	O(r ²)	$c^{2^{\kappa}}$
solving $\hat{\mathbf{S}}_{r}^{(K)}$ in the whole space	$O(r^2n + r^2)$	0 (rn)	$1/\sqrt{n}$
Total	O(rm+Kr ³ +nr ²)	O(rn)	$c^{2^{\kappa}}+1/\sqrt{n}$



19/45

4) SimRank Stability Analysis

DEFINITION 1 (SimRank Condition Number).

For a graph G = (V,E) with Q being its backward transition matrix, let

 $\mathbf{L} \stackrel{def}{=} \mathbf{I}_{n^2} - c \cdot (\mathbf{Q} \otimes \mathbf{Q}).$

The SimRank condition number of G, denoted by $\kappa_{\infty}(G)$, is defined as

 $\kappa_{\infty}(\mathcal{G}) \stackrel{def}{=} \left\| \mathbf{L} \right\|_{\infty} \cdot \left\| \mathbf{L}^{-1} \right\|_{\infty}$

Here, $\|\mathbf{L}\|_{\infty}$ is the maximum absolute row sum of the matrix.



4) SimRank Stability Analysis

★ THEOREM 1. Given a graph G = (V,E), for any damping factor c ∈ (0,1), the SimRank condition number has the following tight bound

$$\kappa_{\infty}\left(\mathcal{G}\right) \leq \frac{1+c}{1-c}$$

- Implications
 - evaluate how stable the similarity is to the perturbations in graphs
 - estimate the accuracy of the ranking results invoked by the iteration error
- Application
 - Actual version: $\mathbf{L} \cdot vec(\mathbf{S}) = (1 c) \cdot vec(\mathbf{I}_n)$

Perturbed version:

$$\tilde{\mathbf{L}} \cdot vec(\tilde{\mathbf{S}}) = (1-c) \cdot vec(\mathbf{I}_n)$$

$$\frac{\left\|\mathbf{S} - \tilde{\mathbf{S}}\right\|_{\max}}{\left\|\tilde{\mathbf{S}}\right\|_{\max}} \le \frac{1+c}{1-c} \cdot \frac{\left\|\tilde{\mathbf{L}} - \mathbf{L}\right\|_{\infty}}{\left\|\mathbf{L}\right\|_{\infty}}.$$

Setting c=0.95 holds the possibility that the relative error in similarity may be (1 + 0.95)/(1 - 0.95) = 40 times larger than the relative error in the link structure. 20/45



4) SimRank Stability Analysis

EXAMPLE 1. The bound of SimRank condition number is tight.



Setting c = 0.7, on one hand,

$$\mathbf{L} = \mathbf{I}_{n^{2}} - c \cdot (\mathbf{Q} \otimes \mathbf{Q})$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} - 0.7 \cdot \left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) = \begin{bmatrix} 1 & 0 & 0 & -.7 \\ 0 & 1 & -.7 & 0 \\ -.7 & 0 & 0 & 1 \end{bmatrix},$$

$$\mathbf{L}^{-1} = \begin{bmatrix} 1 & 0 & 0 & -.7 \\ 0 & 1 & -.7 & 0 \\ 0 & -.7 & 1 & 0 \\ -.7 & 0 & 0 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1.960 & 0 & 0 & 1.373 \\ 0 & 1.960 & 1.373 & 0 \\ 0 & 1.373 & 1.960 & 0 \\ 1.373 & 0 & 0 & 1.960 \end{bmatrix},$$

$$\kappa_{\infty}(\mathcal{G}_{1}) = \|\mathbf{L}\|_{\infty} \cdot \|\mathbf{L}^{-1}\|_{\infty} = 1.7 \times 3.333 = 5.667.$$

On the other hand,

$$\frac{+c}{-c} = \frac{1+0.7}{1-0.7} = 5.667.$$



5.2 SimFusion Overview

Features

- Using a Unified Relationship Matrix (URM) to represent relationships among heterogeneous data
- Defined recursively and is computed iteratively
- Applicable to any domain with object-to-object relationships

Challenges

- URM may incur trivial solution or divergence issue of SimFusion.
- Rather costly to compute SimFusion on large graphs
 - Naïve Iteration: matrix-matrix multiplication
 - Requiring O(Kn³) time, O(n²) space [Xi et. al., SIGIR 05]
- No incremental algorithms when edges update



Existing SimFusion: URM and USM

- ✤ Data Space: $\mathcal{D} = \{o_1, o_2, \cdots\}$ a finite set of data objects (vertices)
- ✤ Data Relation (edges) Given an entire space $\mathcal{D} = \bigcup_{i=1}^{N} \mathcal{D}_i$
 - ♦ Intra-type Relation $\mathcal{R}_{i,i} \subseteq \mathcal{D}_i \times \mathcal{D}_i$ carrying info. within one space
 - ♦ Inter-type Relation $\mathcal{R}_{i,j} \subseteq \mathcal{D}_i \times \mathcal{D}_j$ carrying info. between spaces

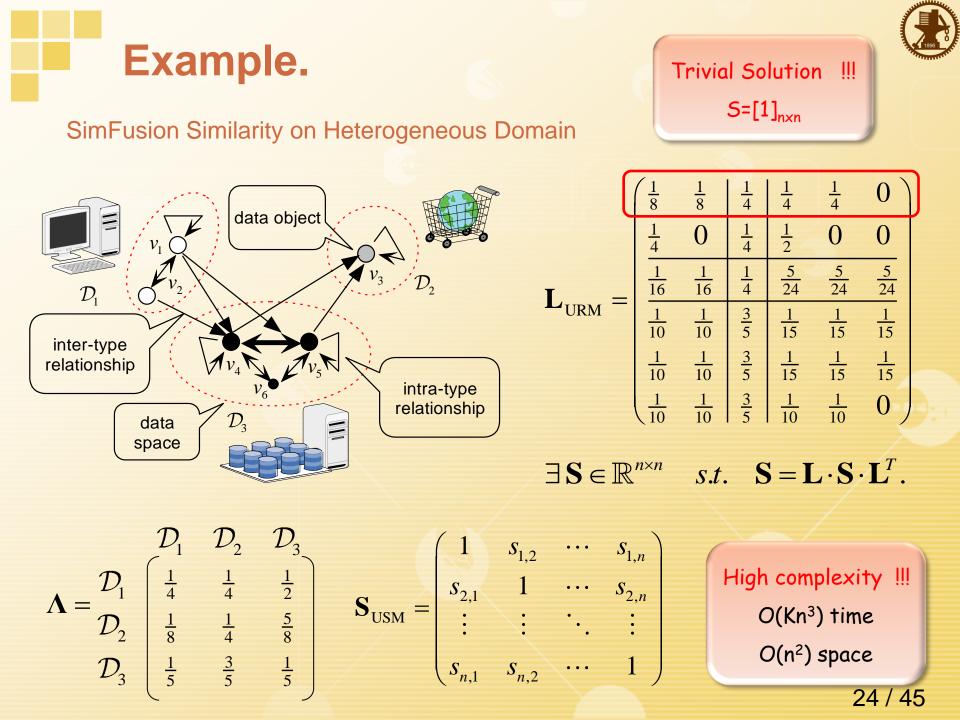
Unified Relationship Matrix (URM):

$$\mathbf{L}_{\text{URM}} = \begin{pmatrix} \lambda_{1,1}\mathbf{L}_{1,1} & \lambda_{1,2}\mathbf{L}_{1,2} & \cdots & \lambda_{1,N}\mathbf{L}_{1,N} \\ \lambda_{2,1}\mathbf{L}_{2,1} & \lambda_{2,2}\mathbf{L}_{2,2} & \cdots & \lambda_{2,N}\mathbf{L}_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{N,1}\mathbf{L}_{N,1} & \lambda_{N,2}\mathbf{L}_{N,2} & \cdots & \lambda_{N,N}\mathbf{L}_{N,N} \end{pmatrix} \qquad \qquad \mathbf{L}_{i,j}(x,y) = \begin{cases} \frac{1}{n_j}, & \text{if } \mathcal{N}_j(x) = \emptyset; \\ \frac{1}{|\mathcal{N}_j(x)|}, & \text{if } (x,y) \in \mathcal{R}_{i,j}; \\ 0, & \text{otherwise.} \end{cases}$$

 $\diamond \lambda_{i,j}$ is the weighting factor between D_i and D_j

Unified Similarity Matrix (USM):

$$\exists \mathbf{S} = \begin{pmatrix} s_{1,1} & \dots & s_{1,n} \\ \vdots & \ddots & \vdots \\ s_{n,1} & \dots & s_{n,n} \end{pmatrix} \in \mathbb{R}^{n \times n} \quad s.t. \quad \mathbf{S} = \mathbf{L} \cdot \mathbf{S} \cdot \mathbf{L}^{T}.$$







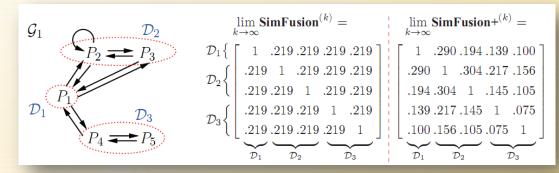
- Revising the existing SimFusion model, avoiding
 - non-semantic convergence
 - divergence issue
- Optimizing the computation of SimFusion+
 - O(Km) pre-computation time, plus O(1) time and O(n) space
 - Better accuracy guarantee
- Incremental computation on edge updates
 - O(δn) time and O(n) space for handling δ edge updates



Revised SimFusion

Motivation: Two issues of the existing SimFusion model

Trivial Solution on Heterogeneous Domain



Divergent Solution on Homogeneous Domain

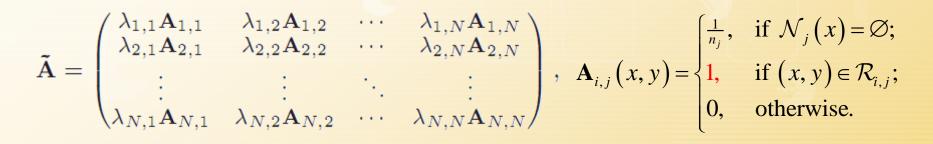
\mathcal{G}_2 P P	$\lim_{k\to\infty} \mathbf{SimFusion}^{(2k)}$	$\lim_{k \to \infty} \mathbf{SimFusion}^{(2k+1)}$	$\lim_{k\to\infty} \mathbf{SimFusion}^{+(k)}$
	$\begin{bmatrix} .46 & 0 & .46 & 0 & .46 \\ 0 & .38 & 0 & .38 & .38 & 0 \end{bmatrix}$	$\begin{bmatrix} .38 & 0 & .38 & 0 & 0 & .38 \\ 0 & .46 & 0 & .46 & .46 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & .25 & 0 & 0 & .25 \\ 0 & 1 & 0 & .25 & .18 & 0 \end{bmatrix}$
P_1 P_6	$.46 \ 0 \ .46 \ 0 \ 0 \ .46 \ \overline{7}$	$\neq \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$.25 \ 0 \ 1 \ 0 \ .25 \ .18 \ 0$
	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$\mathcal{D}_1 \xrightarrow{P_3} \mathcal{P}_5$	$\begin{bmatrix} 0 & .38 & 0 & .38 & .38 & 0 \\ .46 & 0 & .46 & 0 & 0 & .46 \end{bmatrix}$	$\begin{bmatrix} 0 & .40 & 0 & .40 & 0 \\ .38 & 0 & .38 & 0 & 0 & .38 \end{bmatrix}$	$\begin{bmatrix} 0 & .18 & 0 & .23 & 1 & 0 \\ .25 & 0 & .18 & 0 & 0 & 1 \end{bmatrix}$

Root cause: row normalization of URM !!!



From URM to UAM

* Unified Adjacency Matrix (UAM) $A = \tilde{A} + 1/n^2$



Example

$$\Lambda = \begin{bmatrix} \mathcal{D}_{1} \ \mathcal{D}_{2} \ \mathcal{D}_{3} \\ \frac{1}{2} \ \frac{1}{2} \ \frac{1}{6} \ \frac{1}{3} \\ \frac{1}{2} \ \frac{1}{2} \ \frac{1}{4} \\ \frac{1}{3} \ \frac{1}{4} \ \frac{5}{12} \end{bmatrix} \Rightarrow \tilde{\mathbf{A}} = \begin{bmatrix} \frac{1}{2} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \ \frac{1}{12} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \ \frac{1}{12} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \ \frac{1}{12} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ \frac{1}{2} \end{bmatrix} \\ \frac{1}{12} \begin{bmatrix} 1 \\ 2 \\ \frac{1}{2} \end{bmatrix} \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \ \frac{1}{6} \ \frac{1}{6} \ \frac{1}{3} \ 0 \\ \frac{1}{12} \ \frac{7}{12} \ \frac{1}{12} \ \frac{1}{3} \\ \frac{1}{6} \ \frac{7}{12} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{3} \end{bmatrix} \\ \frac{1}{4} \begin{bmatrix} \frac{1}{2} \ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} \\ \frac{1}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \ \frac{1}{6} \ \frac{1}{6} \ \frac{1}{3} \ 0 \\ \frac{1}{6} \ \frac{1}{7} \ \frac{7}{12} \ \frac{1}{8} \ \frac{1}{8} \\ \frac{1}{6} \ \frac{7}{12} \ 0 \end{bmatrix} \\ \frac{1}{6} \ \frac{1}{12} \ \frac{7}{12} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{2} \ \frac{1}{2} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{3} \ \frac{1}{3} \end{bmatrix} \\ \frac{1}{3} \begin{bmatrix} 1 \\ \frac{1}{3} \end{bmatrix} \\ \frac{1}{3} \end{bmatrix} \\$$



Revised SimFusion+

Basic Intuition

replace URM with UAM to postpone "row normalization"
 in a delayed fashion while preserving the reinforcement
 assumption of the original SimFusion

Revised SimFusion+ Model

Original SimFusion

 $\mathbf{S} = \mathbf{L} \cdot \mathbf{S} \cdot \mathbf{L}^T$

$$\mathbf{S} = \frac{\mathbf{A} \cdot \mathbf{S} \cdot \mathbf{A}^{T}}{\|\mathbf{A} \cdot \mathbf{S} \cdot \mathbf{A}^{T}\|_{2}},$$

squeeze similarity scores in S into [0, 1].



Optimizing SimFusion+ Computation

Conventional Iterative Paradigm

$$\mathbf{S}^{(k+1)} = \frac{\mathbf{A} \cdot \mathbf{S}^{(k)} \cdot \mathbf{A}^{T}}{\|\mathbf{A} \cdot \mathbf{S}^{(k)} \cdot \mathbf{A}^{T}\|_{2}}.$$

Matrix-matrix multiplication, requiring O(kn³) time and O(n²) space

Our approach: To convert SimFusion+ computation into finding the dominant eigenvector of the UAM A.

$$[\mathbf{S}]_{i,j} = [\sigma_{\max}(\mathbf{A})]_i imes [\sigma_{\max}(\mathbf{A})]_j$$

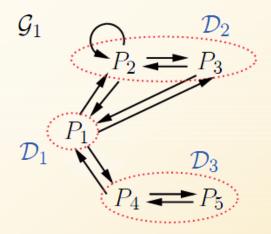
Pre-compute $\sigma_{max}(A)$ only once, and cache it for later reuse

Matrix-vector multiplication, requiring O(km) time and O(n) space

K







Assume $\mathbf{A} = \tilde{\mathbf{A}} + 1/5^2$ with $\tilde{\mathbf{A}} = \begin{bmatrix} \frac{1}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} & \frac{1}{6} \begin{bmatrix} 1 \\ 1 \end{bmatrix} & \frac{1}{3} \begin{bmatrix} 1 \\ 0 \end{bmatrix} & \frac{1}{4} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \\ \frac{1}{6} \begin{bmatrix} 1 \\ 1 \end{bmatrix} & \frac{7}{12} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} & \frac{1}{4} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \\ = \begin{bmatrix} \frac{\frac{1}{2}}{16} & \frac{1}{6} & \frac{1}{3} & 0 \\ \frac{1}{6} & \frac{7}{12} & \frac{1}{2} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{6} & \frac{7}{12} & 0 & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{3} & \frac{1}{6} & \frac{1}{2} & 0 \end{bmatrix} \\ = \begin{bmatrix} \frac{1}{2} & \frac{1}{6} & \frac{1}{6} & \frac{1}{3} & 0 \\ \frac{1}{6} & \frac{7}{12} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{6} & \frac{1}{12} & 0 & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{3} & \frac{1}{8} & \frac{1}{8} & 0 & \frac{5}{12} \\ 0 & \frac{1}{8} & \frac{1}{8} & \frac{5}{12} & 0 \end{bmatrix}$

Conventional Iteration:

$$\mathbf{S}^{(0)} = \mathbf{1} \qquad \mathbf{S}^{(k+1)} = \frac{\mathbf{A} \cdot \mathbf{S}^{(k)} \cdot \mathbf{A}^{T}}{\|\mathbf{A} \cdot \mathbf{S}^{(k)} \cdot \mathbf{A}^{T}\|_{2}} \cdot \mathbf{S} = \begin{bmatrix} .186 & .290 & .194 & .139 & .100 \\ .290 & .453 & .304 & .217 & .156 \\ .194 & .304 & .203 & .145 & .105 \\ .194 & .304 & .203 & .145 & .105 \\ .139 & .217 & .145 & .104 & .075 \\ .100 & .156 & .105 & .075 & .054 \end{bmatrix}$$
$$\mathbf{S}_{1,2} = [\sigma_{\max}(\mathbf{A})]_{1} \times [\sigma_{\max}(\mathbf{A})]_{2} = .431 \times .673 = .290.$$
$$\mathbf{S}_{1,3} = [\sigma_{\max}(\mathbf{A})]_{1} \times [\sigma_{\max}(\mathbf{A})]_{3} = .431 \times .451 = .194.$$



Key Observation

♦ Kroneckor product "⊗":

$$\mathbf{X} \otimes \mathbf{Y} \stackrel{\text{def}}{=} \left[\begin{array}{ccc} x_{1,1}\mathbf{Y} & \cdots & x_{1,q}\mathbf{Y} \\ \vdots & \ddots & \vdots \\ x_{p,1}\mathbf{Y} & \cdots & x_{p,q}\mathbf{Y} \end{array} \right]$$

$$\mathbf{e.g.} \quad \mathbf{X} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}, \quad \mathbf{Y} = \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix}, \quad \mathbf{X} \otimes \mathbf{Y} = \begin{bmatrix} 1 \times \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} & 2 \times \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} & 2 \times \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} = \begin{bmatrix} 5 & 6 & 10 & 12 \\ 7 & 8 & 14 & 16 \\ 15 & 18 & 20 & 24 \\ 21 & 24 & 28 & 32 \end{bmatrix}$$

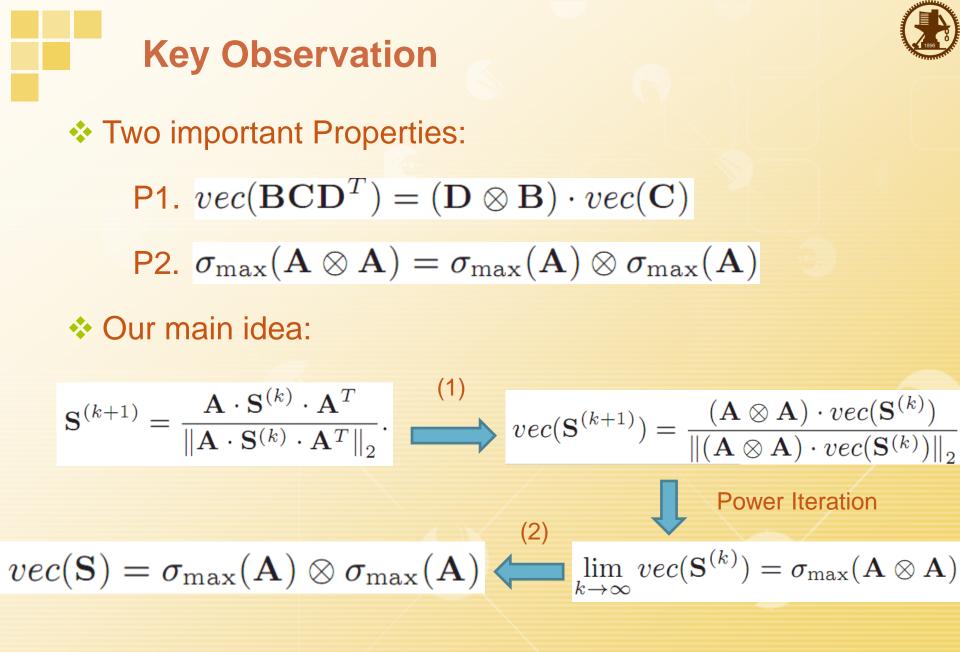
**$$\diamond$$
 Vec operator:** $vec(\mathbf{X}) \stackrel{\text{def}}{=} [x_{1,1}, \cdots, x_{p,1}, \cdots, x_{1,q}, \cdots, x_{p,q}]^T$

e.g.
$$vec(\mathbf{X}) = [1 \ 3 \ 2 \ 4]^T$$

Two important Properties:

$$vec(\mathbf{B}\mathbf{C}\mathbf{D}^T) = (\mathbf{D}\otimes\mathbf{B})\cdot vec(\mathbf{C})$$

$$\sigma_{\max}(\mathbf{A}\otimes\mathbf{A})=\sigma_{\max}(\mathbf{A})\otimes\sigma_{\max}(\mathbf{A})$$



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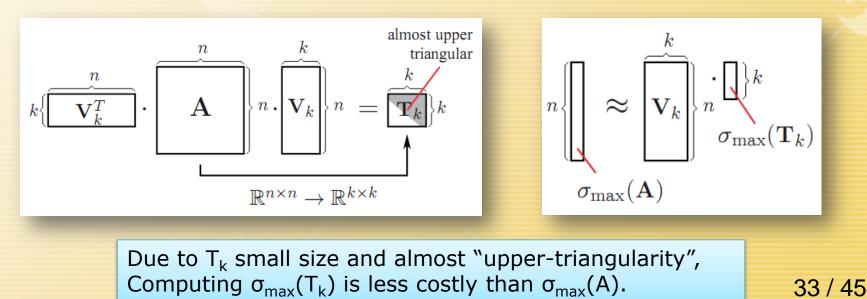
Accuracy Guarantee

Conventional Iterations: No accuracy guarantee !!!

 $\mathbf{S}^{(k+1)} = \frac{\mathbf{A} \cdot \mathbf{S}^{(k)} \cdot \mathbf{A}^{T}}{\|\mathbf{A} \cdot \mathbf{S}^{(k)} \cdot \mathbf{A}^{T}\|_{2}}.$ $\mathbf{S} = \frac{\mathbf{A} \cdot \mathbf{S} \cdot \mathbf{A}^{T}}{\|\mathbf{A} \cdot \mathbf{S} \cdot \mathbf{A}^{T}\|_{2}}$ $\mathbf{Question:} \quad \| \mathbf{S}^{(k+1)} - \mathbf{S} \| \leq \mathbf{?}$

Our Method: Utilize Arnoldi decomposition to build an

order-k orthogonal subspace for the UAM A.



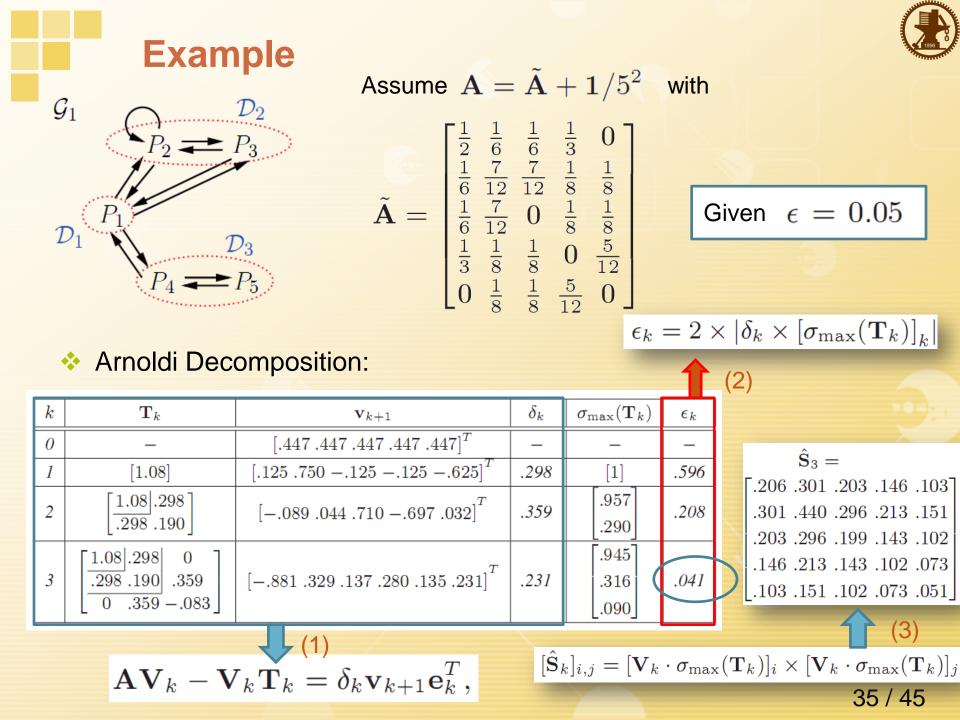


Accuracy Guarantee \diamond Arnoldi Decomposition: $\mathbf{V}_k^T \mathbf{A} \mathbf{V}_k = \mathbf{T}_k$, $\mathbf{V}_k^T \mathbf{A} \mathbf{V}_k = \mathbf{T}_k$, $\mathbf{A} \mathbf{V}_k - \mathbf{V}_k \mathbf{T}_k = \delta_k \mathbf{v}_{k+1} \mathbf{e}_k^T$, $\mathbf{T}_{k+1} = [\mathbf{T}_{\star \star}]$ \diamond k-th iterative similarity

$$[\hat{\mathbf{S}}_k]_{i,j} = [\mathbf{V}_k \cdot \sigma_{\max}(\mathbf{T}_k)]_i \times [\mathbf{V}_k \cdot \sigma_{\max}(\mathbf{T}_k)]_j$$

Estimate Error:

$$\begin{aligned} \|\hat{\mathbf{S}}_{k} - \mathbf{S}\|_{2} &\leq \epsilon_{k} \\ \epsilon_{k} &= 2 \times |\delta_{k} \times [\sigma_{\max}(\mathbf{T}_{k})]_{k} \end{aligned}$$





Edge Update on Dynamic Graphs

Incremental UAM

Given old G = (D,R) and a new G' = (D,R'), the incremental UAM is a list of edge updates, i.e., $\bar{\mathbf{A}} = \mathbf{A}' - \mathbf{A}$

Main idea

To reuse A and the eigen-pair (α_p , ξ_p) of the old A to compute S' A is a sparse matrix when the number δ of edge updates is small.

Incrementally computing SimFusion+

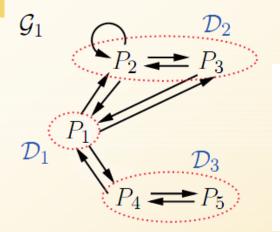
$$[\mathbf{S}']_{i,j} = [\mathbf{\xi}']_i \cdot [\mathbf{\xi}']_j$$
 with $[\mathbf{\xi}']_i = [\mathbf{\xi}_1]_i + \sum_{p=2}^n c_p \times [\mathbf{\xi}_p]_i$

$$c_p = rac{oldsymbol{\xi}_p^T \cdot oldsymbol{\eta}}{lpha_p - lpha_1} \; and \; oldsymbol{\eta} = ar{\mathbf{A}} \cdot oldsymbol{\xi}_1 \; egin{array}{c} \mathsf{O}(\delta n) \; \mathsf{time} \ \mathsf{O}(n) \; \mathsf{space} \end{array}$$

ce







Suppose edges (P1,P2) and (P2,P1) are removed.

	0	$-\frac{1}{6}$	000]
	$-\frac{1}{6}$	0	000
$\bar{\mathbf{A}} =$	0	0	000
	0	0	000
	0	0	000

p	$lpha_p$	$\boldsymbol{\xi}_p$	c_p
1	1.184	$[.431.673.451.322.232]^T$	_
2	.503	$[.708522242 .388 .132]^T$.062
3	480	$\begin{bmatrix}256020 \ .095 \ .716 \641 \end{bmatrix}^T$	018
4	-,366	$\begin{bmatrix}021507 .853119 .017 \end{bmatrix}^T$	025
5	.242	$\left[.497\ .127\ .037\467\719 ight]^T$.069

$$\eta = \bar{\mathbf{A}} \cdot \boldsymbol{\xi}_{1} = \begin{bmatrix} -.112 & -.072 & 0 & 0 \end{bmatrix}^{T}.$$

$$c_{2} = \boldsymbol{\xi}_{2}^{T} \cdot \boldsymbol{\eta} / (\alpha_{2} - \alpha_{1}) = -.0419 / (.503 - 1.184) = .062,$$

$$c_{3} = \boldsymbol{\xi}_{3}^{T} \cdot \boldsymbol{\eta} / (\alpha_{3} - \alpha_{1}) = .030 / (-.480 - 1.184) = -.018$$

$$\boldsymbol{\xi}' = \boldsymbol{\xi}_1 + \sum_{p=2}^{5} c_p \times \boldsymbol{\xi}_p = [.327.703.485.326.266]^T$$

	F .107	.230	.159	.107	.087 .187 .129 .087 .071
	.230	.494	.341	.230	.187
$\mathbf{S}' =$.159	.341	.235	.158	.129
	.107	.230	.158	.107	.087
	[.087]	.187	.129	.087	.071



Experimental Setting

Datasets

- Synthetic data (RAND 0.5M-3.5M)
- Real data (DBLP, WEBKB)

DBLP		$G_1: 01-02$	$G_2: 01-04$	$G_3: 01-06$	$G_4: 01-08$	$G_5: 01-10$
	$ \mathcal{D} $	1,838	3,723	5,772	9,567	12,276
	$ \mathcal{R} $	7,103	14,419	29,054	45,310	64,208

WEBKB

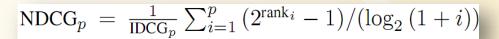
	U_1 : CO	U_2 : TE	U_3 : WA	U_4 : WI
$ \mathcal{D} $	867	827	1,263	1,205
$ \mathcal{R} $	1,496	1,428	2,969	1,805

Compared Algorithms

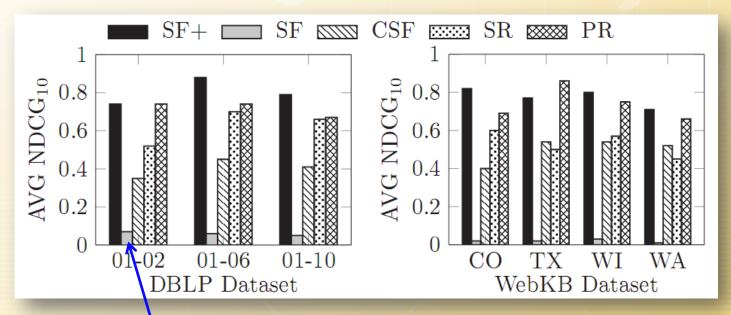
- SimFusion+ and IncSimFusion+ ;
- SF, a SimFusion algorithm via matrix iteration [Xi et. al, SIGIR 05];
- CSF, a variant SF, using PageRank distribution [Cai et. al, SIGIR 10];
- SR, a SimRank algorithm via partial sums [Lizorkin et. al, VLDBJ 10];
- PR, a P-Rank encoding both in- and out-links [Zhao et. al, CIKM 09];



Experiment (1): Accuracy



On DBLP and WEBKB



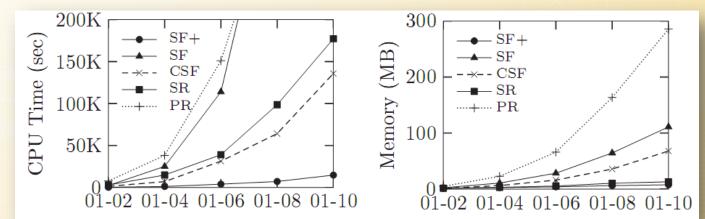
SF+ accuracy is consistently stable on different datasets.

SF seems hardly to get sensible similarities as all its similarities asymptotically approach the same value as K grows.

Experiment (2): CPU Time and Space

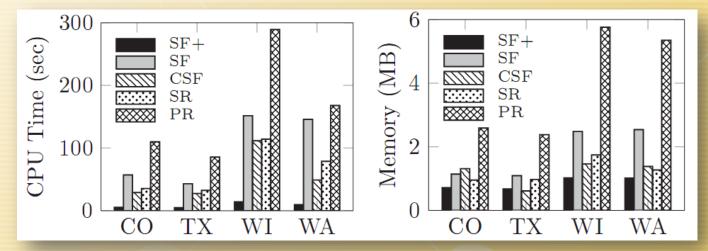


On DBLP



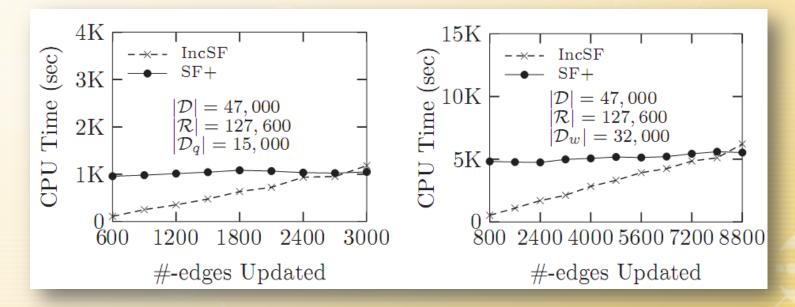
SF+ outperforms the other approaches, due to the use of $\sigma_{max}(T_k)$

On WEBKB



Experiment (3): Edge Updates

Varying **D**

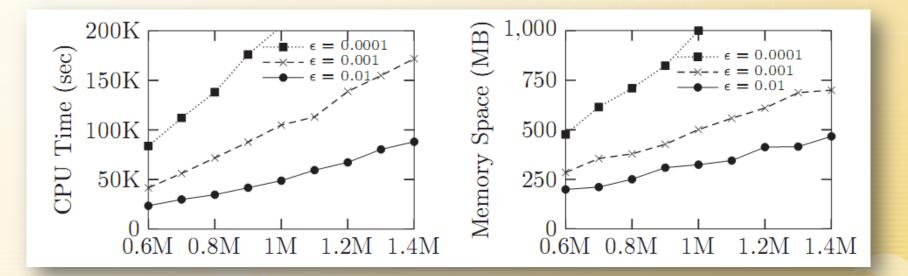


IncSF+ outperformed SF+ when δ is small.

For larger δ , IncSF+ is not that good because the small value of δ preserves the sparseness of the incremental UAM.



Experiment (4) : Effects of ϵ



The small choice of ϵ imposes more iterations on computing T_k and v_k , and hence increases the estimation costs.



Conclusions

- A revision of SimFusion+, for preventing the trivial solution and the divergence issue of the original model.
- Efficient techniques to improve the time and space of SimFusion+ with accuracy guarantees.
- An incremental algorithm to compute SimFusion+ on dynamic graphs when edges are updated.

Future Work

Devise vertex-updating methods for incrementally computing SimFusion+.

Extend to parallelize SimFusion+ computing on GPU.

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Thank You !

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