High Quality SimRank-Based Similarity Search

Weiren Yu and Julie McCann

Department of Computing Imperial College London

Outline

Overview

- The quality of SimRank search
 - Superfluous error
 - Connectivity trait
- Our solutions
 - A "varied-D" method to accurately evaluate SimRank
 - A "kernel-based" model to improve search quality
 - A semantic comparison of two SimRank models
- Experimental Results
- Conclusions

Overview

SimRank in real-world applications:

Customers Who Bought This Item Also Bought







\$299.00



Canon SX40 HS 12.1MP Digital Camera with 35x Wide Angle Optical Image Stabilized Zoom and ...

\$319.76



Sony Cyber-shot DSC-HX200V 18.2 MP Exmor R CMOS Digital Camera with 30x ...

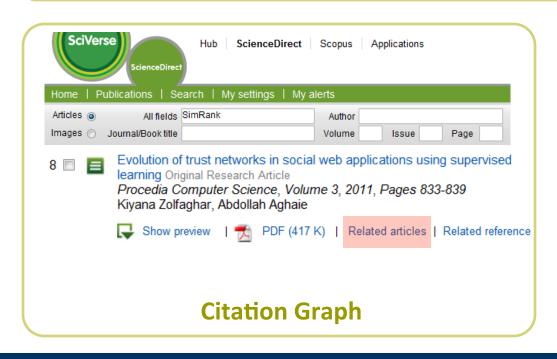
\$348.00



Canon PowerShot SX500 IS 16.0 MP Digital Camera with 30x Wide-Angle Optical ...

\$249.00

Recommender System





SimRank Overview

- SimRank
 - An appealing similarity measure based on graph structure
 - Central idea:

Two nodes are similar if they are pointed to by similar nodes. (recursion)

Each node is most similar to itself. (base case)

- Two formulations of SimRank
 - Jeh and Widom's form (SIGKDD'02)

• Kusumoto et al.'s form

(SIGMOD'14)

in-neighbor set of node *b*

$$S = \max\{\gamma P^{\top} S P, \ I\}$$

Kusumoto et al.'s linearization

Linearized SimRank model:

$$S = \max\{\gamma P^{\top}SP, I\} \Leftrightarrow S = \gamma P^{\top}SP + D$$

Single-pair score S(a,b) can be computed as

$$s(a,b) = e_a^{\top} \underline{D} e_b + \gamma (P e_a)^{\top} \underline{D} (P e_b) + \gamma^2 (P^2 e_a)^{\top} \underline{D} (P^2 e_b) + \cdots$$

However, it is difficult to determine D in advance.

Kusumoto et al.'s approximation

$$D \approx (1 - \gamma)I$$

$$S = \max\{\gamma P^{\top} S P, I\} \Leftrightarrow \tilde{S} = \gamma P^{\top} \tilde{S} P + (1 - \gamma) I$$

Prob 1: Superfluous Diag Error

Two Types of Error:

Exact

$$s(a,b) = e_a^{\top} D e_b + \gamma (P e_a)^{\top} D (P e_b) + \gamma^2 (P^2 e_a)^{\top} D (P^2 e_b) + \cdots$$



$$\epsilon_{\mathrm{diag}} := |s(a,b) - s_{\tilde{D}}(a,b)|$$

Diag Err

Approx. D

$$s_{\tilde{D}}(a,b) = e_a^{\top} \tilde{D} e_b + \gamma (P e_a)^{\top} \tilde{D} (P e_b) + \gamma^2 (P^2 e_a)^{\top} \tilde{D} (P^2 e_b) + \cdots$$



$$\epsilon_{ ext{iter}}:=|s_{ ilde{D}}(a,b)-s_{ ilde{D}}^{(k)}(a,b)|\leq rac{\gamma^{k+1}}{1-\gamma}$$
 Iter Err

K-th Partial Sums

$$s_{\tilde{D}}^{(k)}(a,b) = e_a^{\top} \tilde{D} e_b + \gamma (P e_a)^{\top} \tilde{D} (P e_b) + \dots + \gamma^k (P^k e_a)^{\top} \tilde{D} (P^k e_b)$$

"Iter Err" is convergent when k increases

"Diag Err" is not convergent and sensitive to search quality

Our Method: Varied-D Iteration

- [Kusumoto et al. SIGMOD'14]
 - Hard to determine the exact D in advance

$$S_{\tilde{D}}^{(k)} = \tilde{D} + \gamma P^{\top} \tilde{D} P + \dots + \gamma^{k} (P^{k})^{\top} \tilde{D} P^{k}$$

- Our main idea: Varied-D Model
 - To iteratively compute D and S at the same time

$$S^{(k)} := D_k + \gamma P^{\top} D_{k-1} P + \dots + \gamma^k (P^{\top})^k D_0 P^k$$

When k increases

$$S_{\tilde{D}}^{(k)} \to S_{\tilde{D}} \ (\neq S) \quad (\text{since } \tilde{D} \neq D)$$

$$S^{(k)} \to S$$
 (since $D_k \to D$)



How to iteratively find D_k?

Iteratively Find D_k

D_k can be obtained iteratively as follows:

$$(D_k)_{i,i} = 1 - \sum_{l=1}^k \underbrace{(h_l \circ h_l)^\top} \overrightarrow{diag}(D_{k-l}) \quad with \quad D_0 = I$$
 where
$$\begin{cases} h_0 = e_i \\ h_l = \sqrt{\gamma} P h_{l-1} \end{cases} \quad (l = 1, 2, \cdots, k)$$

• D_k is obtainable in linear memory, independent of $S^{(k)}$ (scalability)

Convergence of Varied-D Model

• Varied-D model to compute S^(k):

$$S^{(k)} := D_k + \gamma P^{\top} D_{k-1} P + \dots + \gamma^k (P^{\top})^k D_0 P^k$$
$$S^{(k)} \to S \qquad \text{(since } D_k \to D\text{)}$$

- How close is S^(k) to S?
 - Our model:

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

No Diag Error, with smaller Iter Error

• Existing work [SIGMOD'14]:

Iter Error



Diag Error

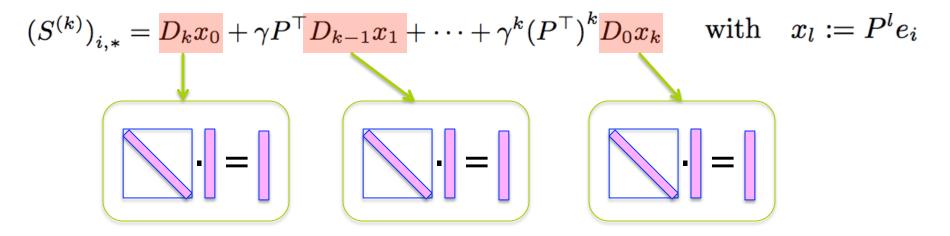
$$\epsilon_{\text{iter}} := |s_{\tilde{D}}(a,b) - s_{\tilde{D}}^{(k)}(a,b)| \le \frac{\gamma^{k+1}}{1-\gamma}$$

$$\epsilon_{\text{diag}} := |s(a, b) - s_{\tilde{D}}(a, b)|$$

Accelerate Computation for Each Column of SimRank

$$S^{(k)} := D_k + \gamma P^{\top} D_{k-1} P + \dots + \gamma^k (P^{\top})^k D_0 P^k$$

Computing i-th column of S^(k)



Accelerate Computation for Each Column of SimRank

$$S^{(k)} := D_k + \gamma P^{\top} D_{k-1} P + \dots + \gamma^k (P^{\top})^k D_0 P^k$$

Computing i-th column of S^(k)

$$(S^{(k)})_{i,*} = D_k x_0 + \gamma P^{\top} D_{k-1} x_1 + \dots + \gamma^k (P^{\top})^k D_0 x_k \quad \text{with} \quad x_l := P^l e_i$$

$$= \begin{bmatrix} + & P^{\top} & P^{\top} & P^{\top} & P^{\top} \end{bmatrix} + \dots$$

Naïve Cost: $O(k^2|E|)$ time [SIGMOD'14]

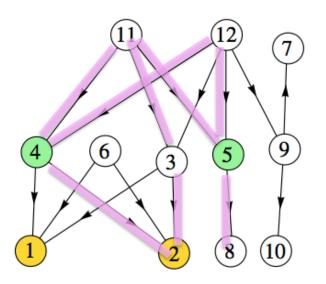
- Our approach
 - multiplying a matrix by a group of vectors added together

$$(S^{(k)})_{i,*} = D_k x_0 + \gamma P^{\top} (D_{k-1} x_1 + \gamma P^{\top} (D_{k-2} x_2 + \cdots + \gamma P^{\top} (D_1 x_{k-1} + \gamma P^{\top} (D_0 x_k))))$$

Our Cost: O(k|E|) time

Prob 2: "Connectivity Trait" of SimRank

- "Connectivity Trait" Problem:
 - increasing # of paths between two nodes, say a and b, would incur a decrease in SimRank s(a, b).



SimRank ignores high connectivity between (2,8)

	SR	SR ⁺⁺	RS	SR [#]
s(1,2) > s(4,5)	X	X	✓	✓
s(2,8) > s(8,10)	X	X	X	✓
s(4,5) > s(3,9)	X	✓	✓	1

Four paths between node pair (2,8):

$$2 \leftarrow 4 \leftarrow \boxed{11} \rightarrow 5 \rightarrow 8, \quad 2 \leftarrow 3 \leftarrow \boxed{11} \rightarrow 5 \rightarrow 8$$
$$2 \leftarrow 4 \leftarrow \boxed{12} \rightarrow 5 \rightarrow 8, \quad 2 \leftarrow 3 \leftarrow \boxed{12} \rightarrow 5 \rightarrow 8$$

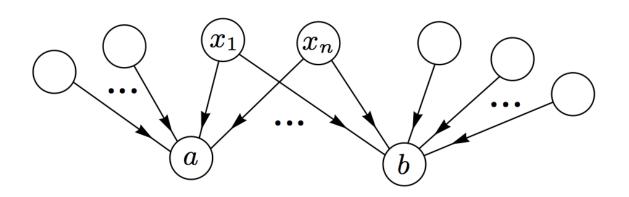
Only one path between node pair (8,10):

$$8 \leftarrow 5 \leftarrow \fbox{12} \rightarrow 9 \rightarrow 10$$

Root Cause of "Connectivity Trait" Issue

$$s(a,b) = \begin{cases} 1 & (a = b) \\ \gamma \cdot \frac{\sum_{(i,j) \in N_a \times N_b} s(i,j)}{|N_a||N_b|} & (a \neq b) \end{cases}$$

• The order of the normalized factor $\frac{1}{|N_a||N_b|}$ is too high.



After δ paths of $\{a \leftarrow x \rightarrow b\}$ are inserted into G:

$$s_{\delta}(a,b) = \gamma \cdot \frac{|N_a \cap N_b| + \delta}{(|N_a| + \delta)(|N_b| + \delta)} \sim \gamma \cdot \frac{\delta}{\delta^2} \to 0. \quad (\delta \to \infty)$$

Our Remedy

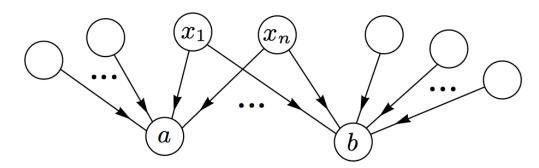
"Cosine-based SimRank" model:

$$\hat{S}_{a,b} = (1 - \gamma) \sum_{k=0}^{\infty} \gamma^k \phi(A^k e_a, A^k e_b) \text{ with } \phi(x, y) := \frac{x^\top y}{\|x\|_2 \|y\|_2}$$

- Main idea:
 - Aggregates weighted cosine similarities between node a's and node b's multi-hop in-neighbor sets
- Advantage:
 - Provides a correct normalized factor for common multihop in-neighbors of a and b

$$\begin{split} \hat{S}_{a,b} &= (1 - \gamma) \sum_{k=0}^{\infty} \gamma^k \frac{|\mathsf{hop}_k(a) \cap \mathsf{hop}_k(b)|}{\sqrt{|\mathsf{hop}_k(a)| \cdot |\mathsf{hop}_k(b)|}} \\ &= (1 - \gamma) \sum_{k=0}^{\infty} \gamma^k \frac{e_a^\top (A^k)^\top A^k e_b}{\|A^k e_a\|_2 \|A^k e_b\|_2} \end{split}$$

Fixing "Connectivity Trait" Issue



After δ paths of $\{a \leftarrow x \rightarrow b\}$ are inserted into G:

Cosine-Based SimRank

$$Ae_a = (\underbrace{1,1,\cdots,1}_{|N_a|},\underbrace{0,0,\cdots 0}_{|N_b-N_a|},\underbrace{1,1,\cdots,1}_{\delta})^{\top} \quad Ae_b = (\underbrace{0,0,\cdots 0}_{|N_a-N_b|},\underbrace{1,1,\cdots,1}_{|N_b|},\underbrace{1,1,\cdots,1}_{\delta})^{\top}$$

$$\hat{S}_{a,b}(\delta) = (1 - \gamma)\gamma \cdot \frac{|N_a \cap N_b| + \delta}{\sqrt{|N_a| + \delta}\sqrt{|N_b| + \delta}} \to (1 - \gamma)\gamma \quad (\delta \to \infty)$$

Naïve SimRank

$$s_{\delta}(a,b) = \gamma \cdot \frac{|N_a \cap N_b| + \delta}{(|N_a| + \delta)(|N_b| + \delta)} \sim \gamma \cdot \frac{\delta}{\delta^2} \to 0. \quad (\delta \to \infty)$$

Semantic Difference of Two SimRank models

Jeh and Widom' model:

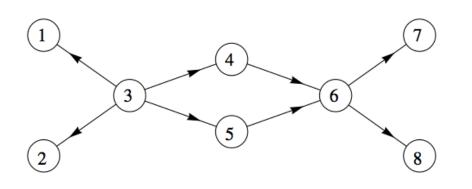
$$S = \max\{\gamma P^{\top} S P, \ I\}$$

• Li et al.'s model:

$$\tilde{S} = \gamma P^{\top} \tilde{S} P + (1 - \gamma) I$$



Any semantic relationship?



node pairs	(3, 3)	(6,6)	 (1, 2)	(7,8)
rank by S	1	1	 9	\overline{g}
$_rank\ by\ ilde{S}$	4	3	 10	9

These two models

- neither yield the same relative rankings,
 [SIGKDD'10]
- 2) nor have the same top-K rankings
 [SIGMOD'14]

Their Semantic Relationship

• Jeh and Widom' model: $S = \max\{\gamma P^{\top}SP, I\}$

$$\Leftrightarrow$$

$$S = I + \gamma (P^{\top}P)_{off} + \gamma^{2} (P^{\top}(P^{\top}P)_{off}P)_{off} + \cdots + \gamma^{k} \underbrace{(P^{\top} \cdots (P^{\top}(P^{\top}P)_{off}P)_{off} \cdots P)_{off}}_{k \ nested \ (*)_{off}} + \cdots$$

Li et al.'s model:

$$\tilde{S} = \gamma P^{\top} \tilde{S} P + (1 - \gamma) I$$

$$\Leftrightarrow$$

$$\frac{\tilde{S}}{1-\gamma} = I + \gamma P^{\top} P + \gamma^2 (P^2)^{\top} P^2 + \dots + \gamma^k (P^k)^{\top} P^k + \dots$$

$$(P^{\top} \cdots (P^{\top} (P^{\top} P)_{off} P)_{off} P)_{off} \cdots P)_{off}$$

$$x_{0} \leftarrow x_{1} \leftarrow \cdots \leftarrow x_{k-1} \leftarrow x_{k} \rightarrow x_{k+1} \rightarrow \cdots \rightarrow x_{2k-1} \rightarrow x_{2k}$$

$$k \ edges$$

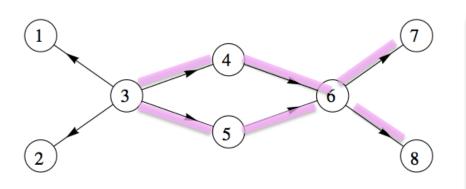
$$k \ edges$$

$$k \ edges$$

$$k \ edges$$

Their Semantic Relationship

k = 1



$$7 \leftarrow 6 \leftarrow 5 \leftarrow \boxed{3} \rightarrow 4 \rightarrow 6 \rightarrow 8$$

- ullet can be tallied by $\left(\left(P^3
 ight)^ op P^3
 ight)$
- but cannot be tallied by

$$(P^{\top}(P^{\top}(P^{\top}P)_{\mathit{off}}P)_{\mathit{off}}P)_{\mathit{off}}P)_{\mathit{off}}$$

k=2

SimRank

k = 0

Li et al.'s model can tally more paths with self-intersected nodes than Jeh and Widom's.

Experimental Settings

Datasets

• Real-life Data:

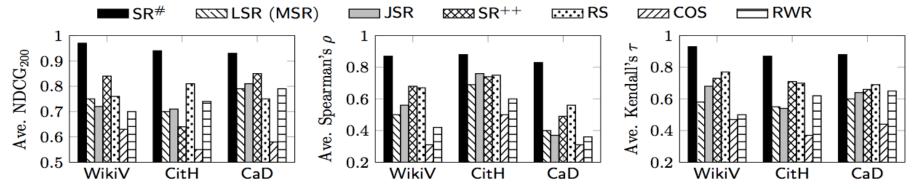
Dataset		E	E / V	Type
WikiV	7,115	103,689	14.57	Directed
CaD	15,683	55,064	5.31	Undirected
CitH	34,546	$421,\!578$	12.20	Directed
WebN	325,729	1,497,134	4.59	Directed
ComY	1,134,890	2,987,624	2.63	Undirected
SocL	4,847,571	68,993,773	14.23	Directed

• Synthetic Data: GraphGen generator

Compared Algorithms

Name	Description
SR [#]	our scheme ("cosine" kernel + computation sharing)
MSR	the state-of-the-art SimRank [7]
OIP	all-pairs SimRank (fine-grained clustering) [13]
PSUM	all-pairs SimRank (partial sums memoization) [12]
SMAT	single-source SimRank (matrix decomposition) [3]
JSR	Jeh and Widom's SimRank [5]
LSR	Li et al.'s SimRank [9]
SR ⁺⁺	SimRank++ (revised "evidence factor") [1]
RS	RoleSim (automorphism equivalence) [6]
RWR	Random Walk with Restart
COS	classic cosine similarity

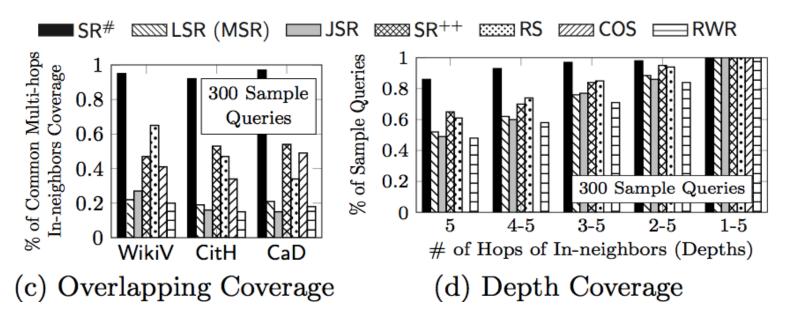
Exp 1: Semantic Quality



(a) Semantics on Real Data (Measured by NDCG, Spearman's ρ , Kendall's τ)

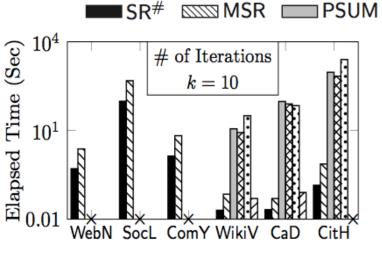
- SR# can avoid "connectivity trait" issue by using a "cosine" kernel.
- COS considers only direct overlapped in-neighbors.
- JSR and LSR both have a "connectivity trait" problem.

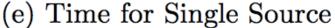
Exp 1: Semantic Quality

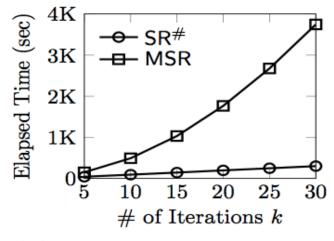


- SR# achieves ~95% coverage of common multi-hop in-neighbors (due to its suitable normalized factor)
- COS (~0.41) consistently outperforms JSR/LSR (~0.20) since COS is not limited by the "connectivity trait" problem.
- The superiority of SR# is more pronounced in the groups with longer paths.

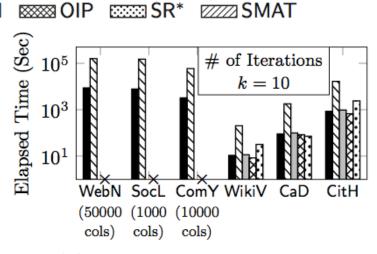
Exp 2: Speedup



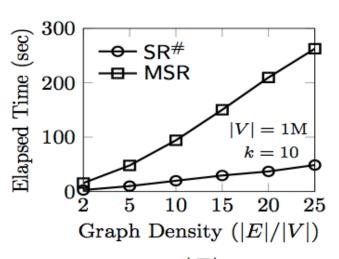




(g) Time vs. k on SocL

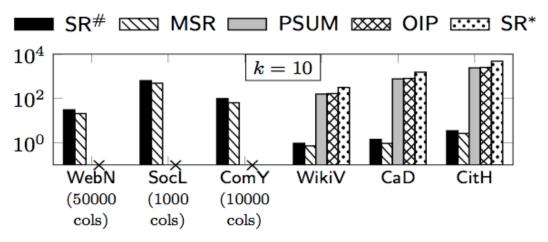


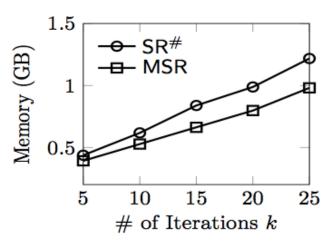
(f) Time for All Pairs



(h) Time $vs. \frac{|E|}{|V|}$ on SYN

Exp 3: Scalability



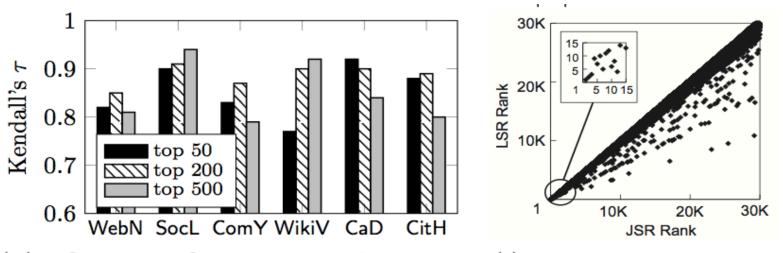


(i) Memory for Single Source/All Pairs

(j) Memory vs. k on SocL

- Only SR# and MSR survive on large datasets, highlighting their scalability.
- The disparity in the memory between SR# and MSR is comparatively small, due to SR# that stores the iterative diagonal correction matrix D_k .

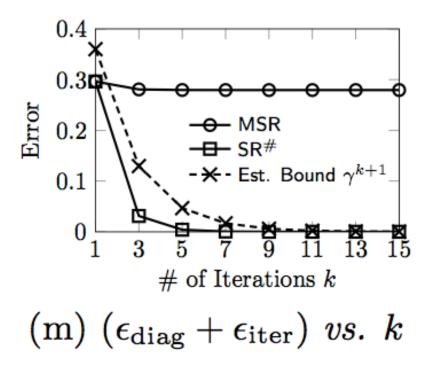
Exp 4: Relative Ordering



(k) LSR and JSR Relative Ordering (l) Ranking on WikiV

- For different graphs, the quality of relative order is irrelevant to top K size.
- LSR does not maintain the relative rank of JSR, even for top 50.
- Many points below the diagonal imply that low-ranked node-pairs by JSR have greater likelihood to get promoted to a high rank of LSR.

Exp 5: Effect of Diag Error



- Our "varied-D" iterative model can guarantee the error to be small and convergent w.r.t k.
- The SR# curve is always below the Est. Bound curve, showing the correctness of our error estimation.

In Conclusion

- We have focused on high quality of SimRank search:
 - Devise a "varied-D" method to remove diagonal error of Kusumoto et al.'s SimRank model
 - Design a "kernel-based" model to resolve connectivity trait problem of SimRank
 - Semantically show the difference between
 Li et al.'s and Jeh et al.'s SimRank models



Existing Link-based Measure

PageRank

$$\mathbf{p} = C \cdot \mathbf{W}^T \cdot \mathbf{p} + (1 - C) \cdot \mathbf{1}$$
 vector of all 1s

Personalized PageRank

$$\mathbf{p} = C \cdot \mathbf{W}^T \cdot \mathbf{p} + (1 - C) \cdot \mathbf{q}$$
 personalized vector

Random Walk with Restart

$$\mathbf{p} = C \cdot \mathbf{W}^T \cdot \mathbf{p} + (1 - C) \cdot \mathbf{e}_i$$
 unit vector

SimRank

$$\mathbf{S} = C \cdot (\mathbf{Q} \cdot \mathbf{S} \cdot \mathbf{Q}^T) + (1 - C) \cdot \mathbf{I}_n$$
 identity matrix
$$\mathbf{S} = C \cdot \mathbf{Q} \cdot \mathbf{S} \cdot \mathbf{Q}^T + \mathbf{D}$$
 diagonal matrix