High Quality Graph-Based Similarity Search

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ABSTRACT

SimRank is an influential link-based similarity measure that has been used in many fields of Web search and sociometry. The best-of-breed method by Kusumoto et al. [7], however, does not always deliver high-quality results, since it fails to accurately obtain its diagonal correction matrix \( D \). Besides, SimRank is also limited by an unwanted "connectivity trait": increasing the number of paths between nodes \( a \) and \( b \) often incurs a decrease in score \( s(a, b) \). The best-known solution, SimRank++, [1], cannot resolve this problem, since a revised score will be zero if \( a \) and \( b \) have no common in-neighbors.

In this paper, we consider high-quality similarity search. Our scheme, \( \text{SR}^\alpha \), is efficient and semantically meaningful:

1. We first formulate the exact \( D \), and devise a "varied-\( D \)" method to accurately compute SimRank in linear memory. Moreover, by grouping computation, we also reduce the time of [7] from quadratic to linear in the number of iterations.
2. We design a "kernel-based" model to improve the quality of SimRank, and circumvent the "connectivity trait" issue. We give mathematical insights to the semantic difference between SimRank and its variant, and correct an argument

\[ s(a, b) = \begin{cases} 1 & (a = b) \\ \gamma \sum_{i,j \in N_a \cap N_b} s(i, j) / |N_a| |N_b| & (a \neq b) \end{cases} \]

where \( \gamma \in (0, 1) \) is a decay factor. Generally, \( \gamma = 0.6 \) [12] or 0.8 [5], which penalizes long paths relative to short ones.

In contrast with other similarity measures, SimRank has the following prominent features: (a) It takes a concise form that captures both direct and indirect neighbors recursively, unlike Bibliographic Coupling and Co-citation that focus only on direct neighbors. (b) It considers structural equivalence of two nodes, whereas Personalized PageRank focuses on reachability from every node to a query. Therefore, SimRank has attracted increasing attention in recent years [3, 4, 12].

1.1 The Quality of SimRank Search

Despite much effort devoted to fast SimRank computation (e.g., [2, 7, 8, 12, 13]), the quality of SimRank search is still less desirable, due to the following two reasons:

1. Superfluous Diagonal Correction Error \( \epsilon_{\text{diag}} \). The best-of-breed SimRank method by Kusumoto et al. [7] is based on the following "linearized SimRank formula":

\[ s(a, b) = e_a^\top D e_b + \gamma (P e_a)^\top D (P e_b) + \gamma^2 (P^2 e_a)^\top D (P^2 e_b) + \cdots \]

where \( D \) is a precomputed diagonal correction matrix, \( e_a \) is a unit vector with a 1 in the \( a \)-th entry, and \( P \) is the column normalized adjacency matrix, with \( P_{a,b} = \begin{cases} 1/|N_a|, & \text{if } (a,b) \in E; \\ 0, & \text{if } (a,b) \notin E. \end{cases} \)

According to [7], before Eq (2) is computed, \( D \) requires to be determined in advance. However, it is too difficult to compute the exact \( D \) (not to mention within linear memory) since SimRank results have a recursive impact on \( D \). Note that even Kusumoto et al. [7] have not obtained the exact \( D \), but simply approximated \( D \) by \( D := (1-\gamma)I \). Consequently, the diagonal correction error is produced:

\[ \epsilon_{\text{diag}} := |s(a, b) - s_{\overline{D}}(a, b)|, \]

To avoid division by 0 in Eq (1), \( s(a, b) = 0 \) if \( |N_a| |N_b| = 0 \).
where \( s_D(a,b) \) is the estimated similarity when \( D \) is replaced by \( \tilde{D} \) in Eq.(2). After \( D \) is estimated, [7] uses an iterative method that sums up only the first \( k \) terms of series \( s_D(a,b) \), denoted as \( s_D^{(k)}(a,b) \). This yields the iterative error:

\[
\epsilon_{iter} := |s_D(a,b) - s_D^{(k)}(a,b)| \leq \frac{\epsilon_{iter}}{1 - \gamma}
\]

Hence, the total error for approximating \( s_D(a,b) \) by \( s_D^{(k)}(a,b) \), in a nutshell, consists of two ingredients: \( \epsilon_{diag} \) and \( \epsilon_{iter} \).

We argue \( \epsilon_{diag} \) is far more serious than \( \epsilon_{iter} \), because \( \epsilon_{iter} \) is guaranteed to converge by [7], and can be minimized by increasing the number of iterations. This increase, however, cannot minimize \( \epsilon_{diag} \). Worse still, there is no bound on \( \epsilon_{diag} \) in Eq.(3). The only argument about \( \epsilon_{diag} \) in [7] is that “estimating \( D \) as \( D := (1 - \gamma)I \) does not much affect the top-K rankings of SimRank++ and RoleSim”, but this, as will be shown in Section 4.1, bears a blemish.

This motivates us to design an accurate and fast approach that has no \( \epsilon_{diag} \) and can avoid computing the exact \( D \).

(2) “Connectivity Trait” Problem. Another factor that plagues the quality of SimRank is the “connectivity trait”: increasing the number of paths between nodes \( a \) and \( b \) often incurs a contrary decrease in \( s(a,b) \). However, a paucity of existing works [1, 2, 11] only noticed a special case (1-hop neighbor) of the above phenomenon: “increasing the number of common in-neighbors between nodes \( a \) and \( b \) will decrease \( s(a,b) \).” The best-known treatment is due to Antonellis et al. who proposed SimRank++ [1] that replaces \( \gamma \) in Eq.(1) with the following “evidence factor”:

\[
\hat{\gamma} := \gamma(1 - e^{-|N_a \cap N_b|}) \quad \text{or} \quad \hat{\gamma} := \gamma \sum_{i=1}^{|N_a \cap N_b|} \frac{1}{i} \quad (4)
\]

These revised “evidence factors” have a good property: \( \hat{\gamma} \) is increasing with respect to \( |N_a \cap N_b| \). Hence, a larger \( \hat{\gamma} \) means that there are more common direct in-neighbors (i.e., more paths of length 2) between \( a \) and \( b \).

However, we observe a weakness of SimRank++ [1]: SimRank++ score \( \tilde{s}(a,b) \) is always zero if nodes \( a \) and \( b \) have no common (direct) in-neighbors. This is because, by the definition in Eq.(4), if \( N_a \cap N_b = \emptyset \), then \( \tilde{s}(a,b) = 0 \). Thus, \( s(a,b) = 0 \), regardless of how many common l-hop in-neighbors (\( l > 2 \)) exist between \( a \) and \( b \).

Other pioneering works (e.g., RoleSim [6], PSimRank [2], and MatchSim [11]) to quantify \( s(a,b) \) also resort to common direct in-neighbors between \( a \) and \( b \), all of which can resolve the special case (1-hop) of the SimRank “connectivity trait” problem (see related work in Section 1.3.2 for more details). However, increasing the number of paths with length \( > 2 \) between \( a \) and \( b \) may still lead to a decrease in \( s(a,b) \).

Example 1. Consider a real Web graph \( G \) in Figure 1. We evaluate the similarity of each node-pair by 4 measures: (a) SR (Jeh and Widom’s SimRank [5]); (b) SR++ (SimRank++ [1]); (c) RS (RoleSim [6]); (d) SR® (our method).

The results are partly depicted in the table. We notice that SR++ and RS do not well resolve the SR “connectivity trait”.

For example, most people may agree \( s(1,2) \) > \( s(4,5) \) since node-pair (1,2) has 3 common in-neighbors [4, 6, 3] whereas (4,5) has only 2 in common [11, 12]. However, although SR++ narrows the gap between \( s(1,2) \) and \( s(4,5) \), it gives the same counter-intuitive answer \( s(1,2) \) < \( s(4,5) \) as SR.

Another example is the comparison of \( s(2,8) \) and \( s(8,10) \). For SR++, \( s(2,8) = s(8,10) = 0 \). This is because (2,8) has no common direct in-neighbors, \( N_2 \cap N_8 = \emptyset \; \text{neither} \; (8,10) \). Their, “evidence factors” \( \hat{\gamma} = 0 \). However, there are 4 indirect path-pairs in-linked from (2,8):

\[
2 \leftrightarrow 4 \leftarrow 11 \rightarrow 5 \rightarrow 8, \quad 2 \leftrightarrow 3 \leftarrow 11 \rightarrow 5 \rightarrow 8
\]

as opposed to only 1 from (8,10): \( 8 \leftrightarrow 5 \leftarrow 12 \rightarrow 9 \rightarrow 10 \).

Thus, (2,8) has a higher connectivity than (8,10), but this connectivity trait is ignored by SR++. Regarding RS, since it is a “role” similarity measure, it emphasizes more on similar node degrees than high connectivities. Thus, RS can only partially resolve the SR “connectivity trait” problem.

Example 1 suggests that the state-of-the-art methods (e.g., SimRank++ [1] and RoleSim [6]) cannot solidly circumvent the “connectivity trait” problem of SimRank. Unfortunately, as illustrated by our statistical experiments in Section 5.2, there are many node-pairs suffering from this problem (e.g., 62.3% in social networks, 82.7% in Web graphs, and 56.4% in citation graphs), which has adversely affected the quality of similarity search. This highlights our need for a high-quality model to resolve the “connectivity trait” problem.

1.2 Our Contributions

Our main contributions are summarized as follows:

- We formulate the exact diagonal correction matrix \( D \), and propose a “varied-\( D \)” method to accurately compute SimRank with no \( \epsilon_{diag} \) and in linear memory. Moreover, by grouping computation, we also optimize the algorithm [7] from quadratic to linear time \( w.r.t. \) \( k \). (Section 2)
- We observe a “connectivity trait” problem for SimRank, which SimRank++ [1] cannot resolve in a recursive style. To circumvent this problem, we design a “kernel-based” model and improve the search quality. (Section 3)
- We give mathematical insights to the semantic difference between Jeh and Widom’s model [5] and its variant [9], and correct an argument [7]: if \( D \) is replaced by \( (1 - \gamma)I \), top-K rankings will not be affected much. (Section 4)

The comprehensive experiments verify that our methods (1) improve an accuracy of average NDCG@200 by \( \sim 30\% \) over SimRank on various real networks, and (2) are \( \sim 10x \) faster than the state-of-the-art competitors on large datasets with 65.8M links for 1000 queries.

1.3 Related Work

1.3.1 SimRank Computation

Recent years have witnessed a surge of efficient methods to compute SimRank. They can be categorized as follows:

- **Single-source SimRank** [3, 7, 8]. Compute all \( s(i,\ast) \).
- **All-pairs SimRank** [9, 12, 13, 16]. Compute all \( s(\ast,\ast) \).
- **Single-pair SimRank** [2, 7, 10]. Compute \( s(i,\ast) \).
Table 1: A comparison with previous deterministic methods
(with low-rank \( r \leq |V| \), degree \( d = \frac{|E|}{|V|} \), and \( d' \leq d \))

In Table 1, we briefly summarize the accuracy, time, and memory of previous works for each type of SimRank search.

Compared with the best-known method [7], our techniques not only preserve the scalability of [7], but also achieve high accuracy and fast computational time. Furthermore, for high-precision methods, our only method not only removes superfluous error \( \epsilon_{\text{diag}} \) but also obtains a better bound on \( \epsilon_{\text{ter}} \) than [7].

### 1.3.2 SimRank “Connectivity Trait”

Fogaras et al. [2] is the first to notice one special case of the SimRank “connectivity trait” problem: “if two nodes \( a \) and \( b \) have \( \beta \) common (direct) in-neighbors, then \( s(a,b) \leq \beta \).” To address this problem, they employed an unwieldy method that divides the entire search space into three probabilities: \( |N_a \cap N_b| \), \( |N_a \cap \bar{N}_b| \), and \( |N_a \cap \bar{N}_b| \). This complicates the revised SimRank equation, which is rather tedious.

Recently, Antonellis et al. [1] gave an excellent revision, called SimRank++, by introducing the “evidence factor” \( \gamma \). Unfortunately, \( \gamma \) can only in, part, alleviate a special case of the “connectivity trait” problem, since, if \( |N_a \cap N_b| = 0 \), then \( \gamma = 0 \) has no recursive impact on SimRank any more.

Jin et al. [6] also gave an excellent exposition on “role similarity”. Their proposed model, namely RoleSim, has the advantage of utilizing “automorphic equivalence” to improve the quality of similarity search in “role” based applications. Their initial intention, however, was not to deal with the SimRank “connectivity trait” problem.

There is also a SimRank-like “connectivity trait” problem in other SimRank variant models, such as MatchSim, SimRank*, SimFusion+ [15]. Our proposed methods for SimRank are also extensible to SimRank*.

Due to space limitation, we omit it in this paper.

### 1.3.3 Semantics between SimRank and Its Variant

There are some interesting works (e.g., [3, 4, 9, 14, 17]), based on the following model, to evaluate similarity \( S \):

\[
S = \gamma P^T SP + (1 - \gamma) I.
\]

[7] argued that “the top-K rankings of \( S \) in Eq.(5) and \( S \) in Eq.(1) are not affected much”. However, we correct this argument, and provide new mathematical insights into the subtle difference of \( S \) and \( S \) from a semantic perspective.

### 2. ACCURATE AND FAST SIMRANK

We first show the sensitivity of diagonal correction matrix \( D \) to SimRank matrix \( S \), and formulate the exact \( D \). Then, we devise an accurate fast “varied-D” model to compute \( S \).

#### 2.1 Sensitivity of Diagonal Correction Matrix

In matrix forms, SimRank in Eq.(1) can be rewritten as

\[
S = \max(\gamma P^T SP, I),
\]

where \( \max(*) \) denotes the matrix entry-wise maximum, i.e., \( (\max(A,B))_{i,j} = \max(A_{i,j},B_{i,j}) \).

Kusumoto et al. [7] have showed that there exists a unique diagonal matrix \( D \) such that Eq.(6) can be converted to

\[
S = \gamma P^T SP + D,
\]

where \( D \) is called the diagonal correction matrix, which needs to be determined beforehand.

However, [7] did not mention how to accurately compute the exact \( D \), but simply approximated \( D \) by \( D = (1 - \gamma)I \).

In fact, \( D \) is very sensitive to the resulting \( S \). Even small errors in \( D \) may lead to large changes in SimRank scores \( S \) by a factor of up to \( \frac{1}{1-\gamma} \), as shown in Lemma 1.

**Lemma 1.** Let \( S \) be the solution to Eq.(7), and \( S_D \) be the solution to the equation:

\[
S_D = \gamma P^T SP + \tilde{D},
\]

and let \( \Delta D := D - \tilde{D} \) and \( \Delta S := S - S_D \). Then,

\[
\|\Delta S\|_\infty \leq \frac{1}{1-\gamma}\|\Delta D\|_\max.
\]

**Proof.** The recursion of \( S_D \) in Eq.(8) naturally leads to the following series:

\[
S_D = \tilde{D} + \gamma P^\top \tilde{D} P + \gamma^2 (P^\top)^2 \tilde{D} P^2 + \cdots.
\]

We subtract Eq.(10) from Eq.(2), and then take \( \|\cdot\|_\max \) norms on both sides:

\[
\|\Delta S\|_\infty \leq \|\Delta D\|_\max + \sum_{i=1}^\infty \gamma^i \|(P^\top)^i \Delta D(P^i)\|_\max
\]

\[
\leq (1 + \gamma + \gamma^2 + \cdots)\|\Delta D\|_\max = \frac{1-\gamma}{1-\gamma}\|\Delta D\|_\max.
\]

#### 2.2 Formulating Diagonal Correction Matrix

We next derive an exact explicit formulation of \( D \) in Eq.(7). For ease of exposition, the following notations are adopted.

**Definition 1 (Entry-Wise Product).** For matrices \( X \) and \( Y \), their entry-wise product \( X \odot Y \) is defined as:

\[
(X \odot Y)_{i,j} = X_{i,j}Y_{i,j}.
\]

Let \( diag(Z) \) be a diagonal matrix whose diagonal entries are those of \( Z \), i.e., \( (diag(Z))_{i,i} = Z_{i,i} \).

Using this notation, Eq.(6) can be represented as

\[
S = \gamma P^T SP + I - \gamma diag(P^T SP).
\]

Due to \( D \) uniqueness, Eqs.(7) and (11) imply that

\[
D = I - \gamma diag(P^T SP).
\]

To formulate the exact \( D \) in Eq.(12) only in terms of \( P \), we introduce the following lemma.

**Lemma 2.** Let \( diag(Z) \) be a column vector of the diagonal entries of \( Z \), i.e., \( (diag(Z))_i = Z_{i,i} \). For two \( n \times n \) matrices \( X \) and \( Y \), and an \( n \times n \) diagonal matrix \( Z \), we have

\[
\overline{diag}(X^\top Z Y) = (X \odot Y)^\top diag(Z).
\]

\( \|\cdot\|_\max \) returns the maximum element of a matrix.
Combining Lemma 2 with Eq.(12), we next formulate

**Theorem 1.** The diagonal correction matrix $D$ in Eq.(7) can be explicitly formulated as

$$\overrightarrow{\text{diag}}(D) = \left( \sum_{k=0}^{\infty} \gamma^k (P^k \circ P^k) \right)^{-T} \vec{1},$$

where $\vec{1}$ is a $|V| \times 1$ vector of all $1$s, and $(*)^{-T} := ((*)^T)^{-1}$.

*Proof.* Taking $\overrightarrow{\text{diag}}(*)$ on both sides of Eq.(2) produces

$$\overrightarrow{\text{diag}}(S) = \overrightarrow{\text{diag}}(D) + \gamma \overrightarrow{\text{diag}}(P^TDP) + \gamma^2 \overrightarrow{\text{diag}}((P^T)^2DP^2) + \cdots.$$ (14)

By SimRank definition Eq.(6), we have $S_{i,i} = 1 \ (\forall i \in V)$, which implies that $\overrightarrow{\text{diag}}(S) = \vec{1}$.

Applying Lemma 2 to the right-hand side of Eq.(14) yields

$$\vec{1} = (I + \gamma(P \circ P) + \gamma^2(P^2 \circ P^2) + \cdots)^{-T} \overrightarrow{\text{diag}}(D),$$ (15)

Since $0 \leq (P \circ P)_{i,j} \leq P_{i,j} \leq 1$, one can readily show that $(I + \gamma(P \circ P) + \gamma^2(P^2 \circ P^2) + \cdots)^{-T}$ is diagonally dominant. Multiplying both sides by its inverse produces Eq.(13). \(\square\)

Theorem 1 characterizes the exact $D$ as an infinite series. Hence, prior to computing $S$, it is too difficult to obtain the exact $D$ in only a finite number of iterations. This tells us that using the method of [7] will inately produce $\epsilon_{\text{diag}}$.

Theorem 1 also implies that the estimation $D \approx (1-\gamma)I$ in [7] is not appropriate for accurately computing $S$ in Eq.(7). This is because replacing $(P^k \circ P^k)$ by $P^k$ in Eq.(13) yields

$$\overrightarrow{\text{diag}}(D) \approx \left( \sum_{k=0}^{\infty} \gamma^k P^k \right)^{-T} \vec{1} = (I - \gamma P)^{-T} \vec{1} \approx (1 - \gamma) \vec{1},$$

which suggests that the approximation $D \approx (1-\gamma)I$ in [7] is equivalent to the approximation $P^0 \approx P^k$. Clearly, most people will not agree that $((P^k)_{i,j})^2 \approx (P^k)_{i,j}$ is reasonable. In Section 4.2, we will further discuss $D \approx (1-\gamma)I$ from the viewpoint of semantics.

One benefit of Theorem 1 is that it narrows the boundaries for the range of $D$ in [7], based on the following corollary.

**Corollary 1.** $(1-\gamma)I \leq D \leq I - \gamma \overrightarrow{\text{diag}}(P^T P)$ \(\dagger\)

*Proof.* Since $0 \leq P_{i,j} \leq 1$, we can readily show that

$$(P \circ P)^k \leq (P^k \circ P^k) \leq P^k.$$ Applying this to Eq.(13) yields

$$\left( \sum_{k=0}^{\infty} \gamma^k P^k \right)^{-T} \vec{1} \leq \overrightarrow{\text{diag}}(D) \leq \left( \sum_{k=0}^{\infty} \gamma^k (P^k \circ P^k) \right)^{-T} \vec{1}.$$ Since $\sum_{k=0}^{\infty} X^k = (I - X)^{-1}$, it follows that $(I - \gamma P)^{-T} \vec{1} \leq \overrightarrow{\text{diag}}(D) \leq (I - \gamma (P \circ P))^{-T} \vec{1}$, which is obtained by applying Lemma 2 on both sides, we obtain the results. \(\square\)

In comparison, the best-known bounds for the range of $D$ in Proposition 2 of [7] (i.e., $(1-\gamma)I \leq D \leq I$) are loose and independent of $P$, which is isolated from graph structures.

### 2.3 A “Varied-D” Iterative Model

Another important consequence of Theorem 1 is to derive an accurate SimRank algorithm without $\epsilon_{\text{diag}}$.

Instead of determining the exact $D$ in advance, our method is to iteratively update $D$ and $S$ at the same time. Precisely, we leverage the “varied-D” SimRank model as follows:

$$S^{(k)} := D_k + \gamma P^T D_{k-1} P + \cdots + \gamma^k (P^T)^k D_0 P^k,$$ (16)

where $\{D_k\}$ is a diagonal matrix sequence (convergent to $D$), which can be iteratively obtained while $S$ is being iterated.

Different from the model Eq.(2) by Kusumoto et al. [7], our “varied-D” model Eq.(16) replaces all $D$s by a convergent sequence $\{D_k\}$. The main advantage of our replacement is that Eq.(16) can avoid determining the exact $D$ beforehand, and thereby, will not produce the superfluous error $\epsilon_{\text{diag}}$.

The correctness of our “varied-D” model can be verified by taking limits $k \to \infty$ on both sides of Eq.(16). As $k \to \infty$, $D_k \to D$ and $S^{(k)} \to S$. Thus, Eq.(16) converges to Eq.(2).

#### 2.3.1 Finding $D_k$ in “Varied-D” Model

The challenging problem in our “varied-D” Eq.(16) is to determine the diagonal matrix $D_k$. Our main idea is based on two observations: (a) $S^{(k)}$ in Eq.(16) can be iterated as

$$S^{(l)} = \gamma P^T S^{(l-1)} P + D_l \quad \text{with} \quad S^{(0)} = D_0.$$ (17)

(b) To ensure $\overrightarrow{\text{diag}}(S^{(l)}) = I$, $D_l$ in Eq.(17) must satisfy

$$D_l = I - \gamma \overrightarrow{\text{diag}}(P^T S^{(l-1)} P).$$ (18)

Coupling these observations, we can compute $D_k$ in Eq.(16).

**Theorem 2.** The diagonal correction matrices in Eq.(16) can be iteratively obtained as follows:

$$(D_k)_{i,i} = 1 - \sum_{l=1}^{k} (h_l \circ h_l)^T \overrightarrow{\text{diag}}(D_{k-l}) \quad \text{with} \quad D_0 = I,$$ (19)

where the auxiliary vectors $h_1, \cdots, h_k$ are derived from

$$\begin{cases} h_0 = e_i \\ h_l = \sqrt{\gamma} P^{l-1} e_i \end{cases} \quad (l = 1, 2, \cdots, k)$$ (20)

*Proof.* First, we derive a complete matrix formula of $D_k$.

By Lemma 2, Eq.(19) can be converted to

$$(D_k)_{i,i} = 1 - \sum_{l=1}^{k} h_l^T D_{k-l} h_l$$ (21)

Successive substitution applied to Eq.(20) yields $h_l = \sqrt{\gamma} P^{l-1} e_i$.

Then, substituting this back into Eq.(21) produces

$$D_k = I - \sum_{l=1}^{k} \gamma \overrightarrow{\text{diag}}(P^{l-1}) D_{k-l}(P^{l-1})$$ (22)

Next, we show that $D_k$ in Eq.(22) satisfies Eqs.(16)–(18). It follows from Eq.(16) that

$$\overrightarrow{\text{diag}}(P^T S^{(k-1)} P) = \overrightarrow{\text{diag}}(\sum_{l=1}^{k-1} \gamma^l (P^{l+1})^T D_{k-l}(P^{l+1}))$$

$$= \overrightarrow{\text{diag}}(\sum_{l=1}^{k-1} \gamma^l (P^{l})^T D_{k-l}(P^{l}))$$

The above equation implies that

$$I - \gamma \overrightarrow{\text{diag}}(P^T S^{(k-1)} P) = I - \sum_{l=1}^{k} \gamma \overrightarrow{\text{diag}}(P^{l}) D_{k-l}(P^{l})$$

Applying Eq.(22) to the right-hand side yields Eq.(18). \(\square\)

**Theorem 2** provides a simple efficient way to compute $D_k$.

**Algorithm 1:** Compute Diagonal Matrix $D_k$

1. initialize $t := 0$, $h_0 := e_i$, $D_0 := I$;
2. for $l := 1, 2, \cdots, k$ do
3. compute $h_l := \sqrt{\gamma} P^{l-1} e_i$;
4. update $t := t + (h_l \circ h_l)^T \overrightarrow{\text{diag}}(D_{k-l})$;
5. return $(D_k)_{1,1} := 1 - t$;

The correctness of Algorithm 1 is verified by Theorem 2. Regarding complexity, we have the following result.

\(\dagger\) The convergence of $S^{(k)}$ will be proved in Section 2.3.2.
Theorem 3. Given the total iteration number \( k = 1, 2, \cdots \), Algorithm 1 is in \( O(k|V|) \) memory and \( O(k(|E| + |V|)) \) time.

In contrast to the linear-memory SimRank method in [7], Theorem 3 implies that our “varied-D” method to compute \( D_k \) will not compromise the scalability of [7] for high quality search, since \( D_k \) can be computed in linear memory as well.

2.3.2 Fast Convergence of “Varied-D” Model

Besides no \( \epsilon_{\text{diag}} \) and no need to precompute the exact \( D \), our “varied-D” model, Eq.(16) also converges faster than [7].

Theorem 4. Let \( S(k) \) and \( S \) be the \( k \)-th iterative and the exact SimRank in Eqs.(16) and (7), respectively. Then,

\[
\|S(k) - S\|_{\text{max}} \leq \epsilon^{k+1}.
\]

Proof. We subtract Eq.(7) from Eq.(17) to obtain, \( \forall k, \)

\[
S(k) - S = \gamma P^T (S(k-1) - S) P + (D(k) - D).
\]

We notice from Eq.(18) that \( S(k)_{i,i} = S_{i,i} = 1, \forall i \in V \).

Thus, when \( i \neq j \), it follows from Eq.(24) that, \( \forall i, j \in V \),

\[
(S(k) - S)_{i,j} = \gamma P^T (S(k-1) - S) P_{i,j}.
\]

By Eq.(1), \( \|I - S\|_{\text{max}} \leq \gamma \). Thus, Eq.(23) holds. \( \square \)

In comparison to the bound \( (\sqrt[k+1]{\epsilon}) \) (see Eq.(10) of [7]), Theorem 4 shows that our “varied-D” model not only eliminates \( \epsilon_{\text{diag}} \), but also has a better bound on \( \epsilon_{\text{iter}} \) than [7]. Thus, our “varied-D” model achieves both high-quality and fast convergence rate at the same time.

2.4 Efficiently Computing \( S(k) \)

Having determined \( D_k \) in our “varied-D” model Eq.(16), we next propose our method to efficiently compute \( S(k) \).

The method [7] requires \( O(k^2|E|) \) and \( O(k^2|V||E|) \) time, respectively, to compute single-source and all-pairs SimRank. If we merely apply the method [7] and replace \( D \) with \( D_k \), then our “varied-D” Eq.(16) to compute \( S(k) \) will retain the same complexity as [7] except with no \( \epsilon_{\text{diag}} \) as follows:

**Procedure 2:** Single-Source “Varied-D” SimRank(i)

1. Initialize \( h := 0 \), \( x := e_i \).
2. For \( l := 1, 2, \cdots, k \) do
3. \( \quad \) update \( h \leftarrow h + \gamma^l (P^T)^l (D_{k-l}) x \), \( x := Px \).
4. Return \( (S(k))_{i,*} := h \).

However, we observe that there exist many duplicate products in [7]. Precisely, to obtain the sums of

\[
(S(k))_{i,*} = D_k x_0 + \gamma P^T (D_{k-1}) x_1 + \cdots + \gamma^k (P^T)^k D_0 x_k,
\]

the method [7] separately computes every \( \gamma^l (P^T)^l (D_{k-l}) x_l \) and then adds them together. Its main limitation is that, to compute any power of \( (P^T) \), [7] has to go through all of the previous powers from scratch. As a result, there are \( l \) matrix-vector products to compute each \( h \) in Line 3, leading to \( k^2 \) products for \( k \) iterations in total.

We now propose an efficient method for Procedure 2, which reduces \( O(k^2|E|) \) to \( O(k|E|) \) time, with no loss of accuracy. Our key observation is that “doing each matrix-vector multiplication separately is equivalent to multiplying a matrix by a group of the resulting vectors added together”. Hence, we rearrange the computation of Eq.(26) as follows:

\[
(S(k))_{i,*} = D_k x_0 + \gamma P^T (D_{k-1}) x_1 + \gamma P^T (D_{k-2}) x_2 + \cdots + \gamma^k P^T (D_0 x_k)
\]

and obtain the result by starting with the innermost brackets and working outwards. In contrast with the method [7], Eq.(27) has only \( O(k) \) matrix-vector products in \( k \) brackets, as opposed to \( O(k^2) \) products in Procedure 2.

Based on Eq.(27), we give an efficient way of Procedure 2.

**Algorithm 3:** Optimized Single-Source SimRank(i)

1. Initialize \( x_0 := e_i \).
2. For \( l := 1, 2, \cdots, k \) do
3. \( \quad \) update \( x_l := Px_{l-1} \).
4. Initialize \( y_0 := \text{diag}(D_0) \circ x_k \).
5. For \( l := 1, 2, \cdots, k \) do
6. \( \quad \) update \( y_l := \text{diag}(D_l) \circ x_{k-l} + \gamma P^T y_{l-1} \).
7. Return \( (S(k))_{i,*} := y_k \).

Algorithm 3 can reduce not only the time of single-source SimRank from \( O(k^2|E|) \) [7] to \( O(k|E|) \), but also the time of all-pairs SimRank from \( O(k^2|V||E|) \) [7] to \( O(k|V||E|) \), since all-pairs SimRank runs \( |V| \) times of single-source SimRank.

3. ENHANCING SIMRANK QUALITY

After the superfluous \( \epsilon_{\text{diag}} \) is avoided, we next focus on the “connectivity trait” problem of SimRank.

3.1 The “Connectivity Trait” Problem

We observe that the root cause of the “connectivity trait” problem is that the order of the normalized factor \( \|x\|_2 \) in the SimRank definition Eq.(1) is too high. To clarify this, let us consider the following situation in Figure 2:

Let \( \delta \) be the number of paths \( a \leftarrow x \rightarrow b \) to be inserted between nodes \( a \) and \( b \). By SimRank definition Eq.(1), after insertions, \( s(a,b) \) will become a function of \( \delta \):

\[
s_\delta(a,b) = \gamma \cdot \frac{|N_a \cap N_b| + \delta}{(|N_a| + \delta)(|N_b| + \delta)} \sim \gamma \cdot \frac{\delta}{\delta} \rightarrow 0. \quad (\delta \rightarrow \infty)
\]

This suggests that, for large \( \delta \), \( s_\delta(a,b) \) behaves like \( (\gamma \cdot \frac{\delta}{\delta}) \), which is eventually decreasing w.r.t. \( \delta \).

3.2 Our Kernel-Based SimRank Model

To avoid the order inconsistency between denominator and numerator in Eq.(28), our goal is to judiciously adjust the order of \( \frac{|N_a \cap N_b|}{(|N_a| + \delta)(|N_b| + \delta)} \) in the SimRank definition. Hence, we rearrange the computation of Eq.(26) as follows:

\[
(S(k))_{i,*} = D_k x_0 + \gamma P^T (D_{k-1}) x_1 + \gamma P^T (D_{k-2}) x_2 + \cdots + \gamma^k P^T (D_0 x_k)
\]

where \( \|x\|_2 := \sqrt{\sum_i |x_i|^2} \) denotes the L₂-norm of vector \( x \).
To prevent division by zero in Eq.(29), we define the $k$-th term of the sums to be 0 if $(A^k)_{a,a}$ or $(A^k)_{a,b} = 0$.

Our cosine-based SimRank $\hat{S}_{a,b}$ integrates weighted cosine similarities between $a$’s and $b$’s multi-hop in-neighbor sets. This can be seen more clearly when we rewrite Eq.(29) as

$$\hat{S}_{a,b} = (1 - \gamma) \sum_{k=0}^{\infty} \gamma^k \phi(A^k e_a, A^k e_b)$$

We call $\phi(x, y)$ a kernel similarity function. In Definition 2, we take $\phi(x, y)$ as the well-known cosine similarity function. The vector $A^k e_a$ (resp. $A^k e_b$) in Eq.(30) collects the information about $k$-hop in-neighbors of node $a$ (resp. $b$). Hence, the term $\phi(A^k e_a, A^k e_b)$ in Eq.(30) evaluates how similar node $a$’s and $b$’s $k$-hop in-neighbor sets are likely to be in terms of the number of length-$k$ paths in-linked from both $a$ and $b$. The factor $\gamma^k$ penalizes connections made with distant $k$-hop-in-neighbors, and $(1 - \gamma)$ normalizes $\hat{S}_{a,b}$ into $[0, 1]$. Thus, $\hat{S}_{a,b}$ not only distills the self-referentiality of SimRank, but also extends a one-step cosine similarity to a multi-step one.

**Theorem 5.** The cosine-based SimRank model in Eq.(29) can circumvent the SimRank “connectivity trait” problem.

**Proof.** Let $\text{hop}_k(x) = \{i \in V | (A^k e_i) > 0 \}$ be the $k$-hop in-neighbor set of node $x$. Then, we have

$$e_a^T (A^k)^T A^k e_b = |\text{hop}_k(a) \cap \text{hop}_k(b)|,$$

$$\|A^k e_a\| = \sqrt{|\text{hop}_k(a)|} \cdot \sqrt{|\text{hop}_k(b)|}.$$  

Plugging these into Eq.(29) produces

$$\hat{S}_{a,b} = (1 - \gamma) \sum_{k=0}^{\infty} \frac{\gamma^k |\text{hop}_k(a) \cap \text{hop}_k(b)|}{\sqrt{|\text{hop}_k(a)|} \cdot \sqrt{|\text{hop}_k(b)|}}$$

(31)

When inserting the following $k$ paths between $a$ and $b$: \[a \leftarrow \cdots \leftarrow a \leftarrow \cdots \leftarrow \cdots \leftarrow a \leftarrow \cdots \leftarrow \cdots \leftarrow b\] (32)

we notice that, only for $k_1 = k_2$, the $k_1$-th term of the series Eq.(31) will be changed to a function of $\delta$:

$$f(\delta) = \gamma^{k_1} \frac{|\text{hop}_{k_1}(a) \cap \text{hop}_{k_1}(b)| + \frac{1}{\sqrt{|\text{hop}_{k_1}(a)|} \cdot \sqrt{|\text{hop}_{k_1}(b)|}}}{\sqrt{|\text{hop}_{k_1}(a)|} \cdot \sqrt{|\text{hop}_{k_1}(b)|}}$$

(33)

To show $f(\delta)$ increases $w.r.t. \delta$, we take $\log(\cdot)$ on both sides, and then use implicit differentiation $w.r.t. \delta$ on both sides:

$$f'(\delta) = f(\delta) \left( - \frac{1}{2 \sqrt{|\text{hop}_{k_1}(a)|} \cdot \sqrt{|\text{hop}_{k_1}(b)|}} - \frac{1}{2 \sqrt{|\text{hop}_{k_1}(a)|} \cdot \sqrt{|\text{hop}_{k_1}(b)|}} \right)$$

Since $f(\delta) > 0$ and $|\text{hop}_{k_1}(a)| \geq |\text{hop}_{k_1}(a) \cap \text{hop}_{k_1}(b)|$ and $|\text{hop}_{k_1}(b)| \geq |\text{hop}_{k_1}(a) \cap \text{hop}_{k_1}(b)|$, we can obtain $f'(\delta) > 0$. Thus, $f(\delta)$ increases $w.r.t. \delta$, which implies that paths (32) insertion will not decrease $\hat{S}_{a,b}$. \(\square\)

Indeed, by using $P e_b = A e_b/\|A e_b\|_1$ to the original SimRank Eq.(2), we notice that both Eqs.(2) and (29) tally the same paths in-linked from $a$ and $b$. The difference is norms $\|\cdot\|_2$ and $\|\cdot\|_1$ used by Eq.(29) and Eq.(2) respectively.

Since the SimRank “connectivity trait” problem is due to the high order of $\frac{1}{\sqrt{|N_a||N_b|}}$ in Eq.(1), it is reasonable for us to prevent its high order by replacing $\|\cdot\|_1$ with $\|\cdot\|_2$ since $\|x\|_2 \leq \|x\|_1$. Moreover, by using $\|\cdot\|_2$, $\hat{S}_{a,b}$ can be correctly normalized into $[0, 1]$. This is because $\phi(\cdot, \cdot) \in [0, 1]$, which indicates that $0 \leq \hat{S}_{a,b} \leq (1 - \gamma) \sum_{k=0}^{\infty} \gamma^k \leq 1$ in Eq.(30).

**Example 2.** Recall the $\delta$ paths $\{a \leftarrow x \rightarrow b\}$ to be added into $G$ in Figure 2. After insertion, $\hat{S}_{a,b}(\delta)$ in Eq.(29) can circumvent the “connectivity trait” problem. This is because

$$A e_a = 1, 1, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1 \rightarrow \delta$$

Thus, $\|A e_a\| = \sqrt{\sum_{i=1}^{10} \delta_i} = \sqrt{|N_a| + \delta}$

Then, we have $(A e_a)^T A e_b = |N_a \cap N_b| + \delta$

Therefore, it follows from Eq.(29) that

$$\hat{S}_{a,b}(\delta) = \frac{(1 - \gamma) \delta}{|N_a| + \delta}$$

(33)

Comparing this with Eq.(28), $\hat{S}_{a,b}(\delta)$ is not eventually decreasing $w.r.t. \delta$, which is due to norm $\|\cdot\|_2$ used in Eq.(29). \(\square\)

In contrast to SimRank++ [1] and PSimRank [2] whose revised weight factors rely only on common $N_a$ and $N_b$, our method Eq.(29), even if $N_a \cap N_b = \emptyset$, can evaluate $s(a,b)$ from common multi-hops neighbors $\text{hop}_k(a) \cap \text{hop}_k(b)$.

To compute the cosine-based SimRank score $\hat{S}_{a,b}$, if $a = b$, Eq.(29) implies $\hat{S}_{a,b} = 1$. If $a \neq b$, we compute $\hat{S}_{a,b}$ as

$$\hat{S}_{a,b} = \frac{\hat{S}_{a,b}(1)}{(1 - \gamma)^{k+1}} \cdot \frac{1}{\text{hop}_k(a) \cap \text{hop}_k(b)}$$

(33)

where the auxiliary vectors $u(k)$ and $v(k)$ are obtained by

$$\begin{cases}
    u(0)^T = e_a \\
    v(0)^T = e_b \\
    u(k)^T = \frac{Au(k-1)}{\|Au(k-1)\|_2} \\
    v(k)^T = \frac{Av(k-1)}{\|Av(k-1)\|_2}
\end{cases}$$

(35)

Eqs.(34)–(35) provide an algorithm to compute $\hat{S}_{a,b}^{(k)}$, which is in $O(k|E|)$ time and $O(|E| + k|V|)$ memory for $k$ iterations.

### 4. SEMANTIC DIFFERENCE

Apart from Jeh and Widom’s SimRank model [5]:

$$\hat{S} = \max_{P \in \mathbb{P}} (\gamma P^T S, I),$$

recent years have witnessed many studies (e.g., [3, 4, 9, 14]) to compute similarity, based on Li et al.’s model [9]:

$$\hat{S} = \gamma P^T S + (1 - \gamma) I.$$  

(37)

In this section, we explore their relationship from a semantic perspective, and correct two arguments in [9] and [7].

#### 4.1 A Fly in the Ointment of [7,9]

There are only two works [7,9] that have mentioned the relationship between $\hat{S}$ and $S$. (a) Li et al. [9] argued that “$\hat{S}$ affects only the absolute similarity value of $S$, but not the relative similarity ranking of $S$. “ (b) The recent work by Kusumoto et al. [7] states that “$\hat{S}$ does not much affect the top-k ranking of $S$. ” However, either of them implies a limitation, as disproved by the following counterexample.

**Example 3.** Consider graph $G$ in Figure 3, for $\gamma = 0.6$, the top-10 similarity rankings by $S$ and $\hat{S}$ are shown in part:

<table>
<thead>
<tr>
<th>node pairs</th>
<th>(3, 3)</th>
<th>(6, 6)</th>
<th>(1, 2)</th>
<th>(7, 8)</th>
</tr>
</thead>
<tbody>
<tr>
<td>rank by $S$</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>9</td>
</tr>
<tr>
<td>rank by $\hat{S}$</td>
<td>4</td>
<td>3</td>
<td>9</td>
<td>10</td>
</tr>
</tbody>
</table>

\(\text{In essence, } \hat{S} \approx \hat{S} \text{ is equivalent to } D \approx (1 - \gamma) I.\)
4.2 Semantic Relationship Between $S$ and $\tilde{S}$

To “rekindle” the semantic relationship between $S$ and $\tilde{S}$, let us first introduce the following notation:

**Definition 3** (Off-Diagonal Operator). For square matrix $X$, let $(\ast)_{\text{off}}$ be a matrix operator defined by

$$(X)_{\text{off}} := X - \text{diag}(X).$$

This notation is introduced to bring new insights into $S$.

**Theorem 6.** The similarity $S$ in Jeh and Widom’s model Eq.(36) can be characterized as follows:

$$S = I + \gamma (P^T P)_{\text{off}} + \gamma^2 (P^T (P^T P)_{\text{off}} P)_{\text{off}} + \cdots + \gamma^k (P^T \cdots (P^T P)_{\text{off}} P)_{\text{off}} \cdots P)_{\text{off}} + \cdots$$

**Proof.** Applying $(\ast)_{\text{off}}$, Eq.(36) can be iterated as

$$S_k = \gamma (P^T S_{k-1})_{\text{off}} + I.$$  \hspace{1cm} (39)

We now construct the iterations: starting with $R_0 = I$,

$$R_k = \gamma^k (P^T \cdots (P^T (P^T P)_{\text{off}} P)_{\text{off}} \cdots P)_{\text{off}} + R_{k-1}.$$  \hspace{1cm} (40)

Using induction on $k$, we next show that $S_k = R_k$ ($\forall k$). Clearly, $S_0 = R_0$. Assume $S_k = R_k$ holds, we consider

$$S_{k+1} = \gamma (P^T S_k)_{\text{off}} + I$$  \hspace{1cm} (using the hypothesis $S_k = R_k$)

$$= \gamma^k (P^T \cdots (P^T (P^T P)_{\text{off}} P)_{\text{off}} P)_{\text{off}} + \gamma (P^T R_{k-1})_{\text{off}} + I$$

$$= \gamma^k (P^T \cdots (P^T (P^T P)_{\text{off}} P)_{\text{off}} \cdots P)_{\text{off}} + R_{k+1}.$$  \hspace{1cm} (k+1) nested $(\ast)_{\text{off}}$

By Theorem 6, $S$ in Eq.(36) is the weighted sums of

$$(P^T \cdots (P^T (P^T P)_{\text{off}} P)_{\text{off}} \cdots P)_{\text{off}}$$  \hspace{1cm} $\forall k = 1, 2, \cdots$ \hspace{1cm} (41)

In contrast, $\tilde{S}$ in Eq.(37) is the weighted sums of the terms

$$(P^T \cdots (P^T (P^T P) P) \cdots P)$$  \hspace{1cm} $\forall k = 1, 2, \cdots$ \hspace{1cm} (42)

To find out the semantic difference between $S$ and $\tilde{S}$, we merely need to compare the paths tallied by (41) and (42):

**Theorem 7.** Given a graph $G$, the terms in Eq.(41) tally the following paths in $G$:

$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_{k-1} \leftarrow x_k \rightarrow x_{k+1} \rightarrow \cdots \rightarrow 2k - 1 \rightarrow x_{2k} \rightarrow x = x_{2k+1}$$  \hspace{1cm} (43)

where $x_0, \cdots, x_{2k}$ can be any nodes, but with no repetition of nodes $x_i$ and $x_{2k-i}$ allowed, $\forall i \in \{0, 1, \cdots, 2k\} \setminus \{k\}$.

In comparison, the terms in Eq.(42) tally the paths of (43) in $G$ without having such a constraint on nodes $x_i$ and $x_{2k-i}$.

**Proof.** By the power property of the adjacency matrix, $(P^k)_{\text{off}}$ tallies the paths of (43) between $i$ and $j$.

To show the terms in Eq.(41) tally the paths of (43) with the additional constraint, we use induction on $k$ as follows.

When $k = 1$, $(P^T P)_{\text{off}}$ tallies $x \leftarrow x_j \rightarrow x_i$, and $x_{2k+1}$.

**Example 4.** Recall the graph in Figure 3. By Theorem 7, the path $7 \leftarrow 6 \leftarrow 5 \leftarrow 3 \rightarrow 4 \rightarrow 6 \rightarrow 8$ is tallied by the term $(P^3)_{\text{off}}$, but not by $(P^T (P^T P)_{\text{off}} P)_{\text{off}}$. Indeed, regarding the term $(P^T (P^T P)_{\text{off}} P)_{\text{off}}$, the innermost $(\ast)_{\text{off}}$ disallows paths with repetition of nodes 5 and 4; the second nested $(\ast)_{\text{off}}$ disallows the repetition of nodes 6 and 7 (which is considered the path violates); the outermost $(\ast)_{\text{off}}$ disallows the repetition of nodes 7 and 8.

In light of Theorem 7, the semantic relationship between $S$ and $\tilde{S}$ is evident: $\tilde{S}$ often aggregates more paths than $S$, and $S$ excludes the paths with self-intersecting nodes that are considered by $\tilde{S}$. Figure 4 depicts an illustrative comparison of the paths tally by $(S_k)_{i,j}$ and $(\tilde{S}_k)_{i,j}$ for $k = 0, 1, 2$.

For verification, let us apply $(\ast)_{\text{off}}$ definition to expand, e.g., the term $(P^T (P^T P)_{\text{off}} P)_{\text{off}}$ as follows:

$$((P^T (P^T P)_{\text{off}} P)_{\text{off}})_{i,j} = ((P^2)^T P^2)_{i,j} - (P^T \text{diag}(P^T P) P)_{i,j} - (\text{diag}(P^2) P^2)_{i,j} + (\text{diag}(P^T \text{diag}(P^T P) P))_{i,j}$$

where a circled number beneath each term is associated with a path numbered in the upper-left corner of Figure 4.
The following result shows the specific types of paths that are tallied by \( S \) but not by \( \tilde{S} \).

**Corollary 2.** Let \( \mathcal{P}(S) \) and \( \mathcal{P}(\tilde{S}) \) be the sets of paths tallied by \( S \) and \( \tilde{S} \), respectively. Then, \( \mathcal{P}(\tilde{S}) \supseteq \mathcal{P}(S) \), and \( \mathcal{P}(\tilde{S}) - \mathcal{P}(S) \) is the set of “special” cycles of length \( 2k \) (\( k = 1, 2, \ldots \)), with first \( k \) contiguous edges oriented in one direction, and next \( k \) contiguous edges in the opposite direction.

# 5. EXPERIMENTAL STUDIES

## 5.1 Experimental Setting

### (1) Real Data

| Dataset | \(|V|\) | \(|E|\) | \(|E|/|V|\) | Type |
|--------|--------|--------|-------------|------|
| WikiV  | 7,115  | 143,689 | 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 |

(a) WikiV, a Wikipedia who-votes-on-whom graph, where nodes are users, and an edge \( i \rightarrow j \) means user \( i \) voted on \( j \).

(b) CaD, a collaboration graph, where each node is an author, and edges co-authorships. The graph is derived from 6-year publications (2006-2011) in seven major conferences.

(c) CitH, a citation graph from arXiv high energy physics theory, where each node is a paper labeled with meta information (e.g., title, authors, abstract) and an edge a citation.

(d) WebN, a web graph from University of Notre Dame, where a node is a page (from nd.edu) and an edge a link.

(e) ComY, an undirected Youtube social graph, where a node is a user and an edge a friendship.

(f) SocL, a friendship graph of a LiveJournal community, where \( i \rightarrow j \) is a recommendation of user \( j \) from user \( i \).

### (2) Synthetic Data

To produce SYN, we adopt a scale-free graph generator based on the Barabasi-Albert model. This generator takes as input two parameters: \(|V|, |E|\).

### (3) Query Generator

(i) To evaluate all pairs \( s, t \), we generate the query-pair set \((A, B)\), by using two criteria:

(a) **Importance coverage** is to ensure the selected \((A, B)\) to comprehensively contain a broad range of any possible pairs. To this end, we first sort all nodes in \( V \) in descending order by PageRank (PR), and split them into 10 buckets: nodes with \( PR \in [0.9, 1] \) are in the first bucket; nodes with \( PR \in [0.8, 0.9] \) the second, etc. We next randomly select \( \left\lceil \frac{|A|}{10} \right\rceil \) nodes from each bucket to \( A \) (resp. \( \left\lfloor \frac{|B|}{10} \right\rfloor \) nodes from each bucket to \( A \) (resp. \( B \)). Thus, \((A, B)\) has both important and non-important pairs.

(b) **Overlapping coverage** is to ensure that \((A, B)\) contains node-pairs with many multi-hop in-neighbors overlapped. To achieve this, we first sort node-pair \((a, b)\) in descending order via a scoring function:

\[ f_{a,b} := \sum_{k=1}^{5} \text{hop}_k(a) \cap \text{hop}_k(b) \]

We then split all pairs into 5 buckets: pairs with \( f_{a,b} \in [4, 5] \) are in the first bucket; pairs with \( f_{a,b} \in [3, 4] \) the second, etc. For each bucket, we next sort node-pair \((a, b)\) in descending order based on the value of \( g_{a,b} := \sum_{k=1}^{5} \text{hop}_k(a) \cap \text{hop}_k(b) \), and select top \( \left\lceil \frac{|A|}{5} \right\rceil \) node-pairs from each bucket. Hence, \((A, B)\) covers node-pairs with many multi-hop in-neighbors in common.

(ii) Similarly, to evaluate single-source \( s(q, g) \), the query set for \( g \) can be sampled as “importance coverage”.

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9 http://snap.stanford.edu/data/index.html
10 http://graphstream-project.org/doc/Generators/
11 http://academic.research.microsoft.com/VisualExplorer
12 For semantics evaluation, MSR produces the same similarity values as LSR, since \([7]\) approximates \( D \) by \((1 - \gamma)I\).
To further evaluate the search depth of $SR^*$, $SR^{++}$, $JSR$, $LSR$, $RS$, $COS$, $RWR$, we first apply overlapping coverage criterion to generate 2,000 queries, and then generate 300 queries via importance coverage criterion, and classify them into 4 groups, e.g., “4–5” collects queries $(a, b)$ whose path length between $a$ and $b$ is 8–10. Fig. 5d depicts the search depth of all the methods on WikiV. (1) For each group, $SR^{++}$ and $COS$ have the lowest quality of depth search among all the methods, since they cannot capture the paths of length > 2 between nodes. (2) $SR^*$ achieves the highest quality, and its superiority is more pronounced in the groups that have longer paths. This tells us that the “connectivity trait” issue has a large influence on node-pairs with long paths.

5.2.2 Time Efficiency

Fig. 5e illustrates the running time of $SR^*$, $MSR$, $PSUM$, $OIP$, $SR^*$, $SMAT$ for single-source $s(q)$ on 6 real datasets. (1) In all cases, $SR^*$ always substantially outperforms the other methods. This is because $SR^*$ can eliminate duplicate computations for maximal sharing, whereas $MSR$ computes each term separately. (2) $PSUM$, $OIP$, $SR^*$, $SMAT$ will crash on large WikiV, CitH, ComY, due to the memory allocation. On WikiV and CaD, they are 3–4 orders of magnitude slower than $SR^*$ since their iterative models to compute $s(q)$ rely on all-pairs outputs of the previous iteration.

Fig. 5f shows the time of $SR^*$, $MSR$, $PSUM$, $OIP$, $SR^*$ for all-pairs $s(q)$ on 6 real datasets. (1) Only $SR^*$, $MSR$ survive on all datasets, whereas $PSUM$, $OIP$, $SR^*$ fail on large datasets.
WebN, SocL, ComY, due to the memory allocation. (2) MSR is slower than others as it sacrifices speed for scalability. In contrast, SR\# not only scales well on large graphs, but also has comparable speed to those of PSUM, OIP, SR\#.

Fig. 5g presents the impact of the iteration number \(k\) on the time of SR\# and MSR. When \(k\) grows from 5 to 30, the time of SR\# does not increase significantly (just from 42s to 301s), as opposed to the time of MSR growing from 152s to 3744s. The reason is that MSR contains many duplicate computations among different iterations, whereas SR\# can merge these results after rearranging the computation order. It is consistent with our analysis in Subsection 2.4.

Fig. 5h demonstrates the impact of network density on the computational time of SR\# and MSR on synthetic data. Fixing \(|V| = 1,000,000\) and \(k = 10\), we generate a synthetic dataset by increasing the graph density from 2 to 25. (1) When the density increases, the time of both algorithms will increase. (2) For dense graphs, the speedup for SR\# is significantly higher than MSR, due to the number of iterations with a huge influence on MSR compared with SR\#. This is in agreement with the complexity of SR\# and MSR.

### 5.2.3 Memory Efficiency

Fig. 5i shows the memory of SR\#, MSR, PSUM, OIP, SR\# on six real datasets. (1) For large WebN, SocL and ComY, only SR\# and MSR survive, highlighting their scalability. (2) For each dataset, SR\# requires slightly more memory than MSR because it requires to store \(D_k\).

Fig. 5j statistically shows the percentage of node-pairs with the “connectivity trait” problem over all real datasets. From the results, we see that the percentages are all high (e.g., 82.7% on WebN, 62.3% on SocL, 78.1% on ComY), showing the seriousness of this problem in real scenarios.

### 6. CONCLUSIONS

We consider the problem of high-quality similarity search. Observing that (1) the best-of-breed SimRank [7] produces diagonal correction error \(\epsilon_{\text{diag}}\) and (2) SimRank++ [1] does not well resolve the “connectivity trait” problem, we proposed our scheme, SR\#. First, we characterize the exact \(D\), and devise a “varied-\(D\)” model to compute SimRank with no \(\epsilon_{\text{diag}}\) in linear memory. We also speed up the computational time from quadric [7] to linear in terms of \(k\). Next, we devise a “kernel-based” model to circumvent the “connectivity trait” problem. Finally, we give new insights into the semantic difference between Jeh and Widom’s SimRank and its variant, and correct an argument in [7]. We empirically show that SR\# (1) improves an accuracy of average NDCG@500 by \(\approx 30\%\) on real graphs, and (2) can be \(\approx 10\times\) faster than [7] on SocL with 65.8M links for 1000 queries.

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### 7. REFERENCES