ASAP: Towards Accurate, Stable and Accelerative Penetrating-Rank Estimation on Large Graphs

Xuefei Li[1], Weiren Yu[2,3], Bo Yang[3], and Jiajin Le[3]

[1] Fudan University, China
xuefei.li89@gmail.com
[2] University of New South Wales & NICTA, Australia
weirenyu@cse.unsw.edu.au
[3] Donghua University, China
{yangbo,lejiajin}@dhu.edu.cn

Abstract. Pervasive web applications increasingly require a measure of similarity among objects. Penetrating-Rank (P-Rank) has been one of the promising link-based similarity metrics as it provides a comprehensive way of jointly encoding both incoming and outgoing links into computation for emerging applications. In this paper, we investigate P-Rank efficiency problem that encompasses its accuracy, stability and computational time. (1) We provide an accuracy estimate for iteratively computing P-Rank. A symmetric problem is to find the iteration number K needed for achieving a given accuracy ϵ. (2) We also analyze the stability of P-Rank, by showing that small choices of the damping factors would make P-Rank more stable and well-conditioned. (3) For undirected graphs, we also explicitly characterize the P-Rank solution in terms of matrices. This results in a novel non-iterative algorithm, termed ASAP , for efficiently computing P-Rank, which improves the CPU time from $O(n^4)$ to $O\left(n^3\right)$. Using real and synthetic data, we empirically verify the effectiveness and efficiency of our approaches.

1 Introduction

The study of quantifying structural similarity between vertices in ubiquitous networks has attracted considerable attention over the past decade. Typical structural similarity metrics include Google PageRank, Hyperlink-Induced Topic Search (HITS), Cocitation, Bibliographic Coupling, SimRank and SimFusion (*e.g.,* [1,2,3,4,5,6]).

P-Rank (Penetrating-Rank) is a new similarity measure of this kind, which was initially proposed by Zhao *et al.* [7]. The similarity scores flowing from in-link neighbors of entities are penetrated through their out-link neighbors. Emerging real-world applications of P-Rank include biological networks, collaborative filtering, graph classification, web document ranking, and outlier detection (*e.g.,* [8,9,4,10,5,6]).

In contrast to other similarity measures, P-Rank has become one of the important metrics owing to the following two reasons. (i) P-Rank provides a comprehensive way to jointly explore both in- and out-link relationships with semantic completeness. In comparison, other similarity measures, say SimRank, have the "limited information problem" [5], in which only in-link relationships can be partially exploited. (ii) P-Rank transcends other similarity measures in its most general form. Other measures such as SimRank [5], Amsler [1] can be regarded as just special cases of P-Rank [7].

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Unfortunately, previous work on P-Rank suffers from the following limitations. (i) P-Rank solution is known to converge [7], but a precise accuracy estimation of P-Rank is not given. (ii) No prior work has well studied *the P-Rank condition number*, which indeed has played a paramount role in measuring how much the web graph can change in proportion to small changes in the P-Rank scoring results. (iii) The P-Rank time complexity in [7] retains *quartic* in the worst case for both digraphs and undirected graphs. To the best of our knowledge, there is no efficient P-Rank algorithm specially designed for *undirected graphs*. These practical needs call for an in-depth investigation of P-Rank and its efficiency.

Contributions. This paper studies the P-Rank problems regarding its *accuracy*, *stability* and *computational efficiency*. Our main results are summarized below.

1. We provide an accuracy estimation for P-Rank iteration (Section 3). We find that the number of iterations $K = \lceil \log \epsilon / \log (\lambda \cdot C_{\text{in}} + (1-\lambda) \cdot C_{\text{out}}) \rceil$ suffices to acquire a desired accuracy of ϵ, where λ is a weighting factor, and C_{in} and C_{out} are in- and out-link damping factors, respectively.
2. We introduce the notion of P-Rank *condition number* κ_∞ to investigate the stability issue of P-Rank (Section 4). We show that P-Rank is *well-conditioned* for small choices of the damping factors, by providing a tight *stability bound* for κ_∞.
3. We propose a novel *non-iterative* $O(n^3)$-time algorithm (ASAP) for efficiently computing similarities over undirected graphs (Section 5). We explicitly couch the P-Rank solution *w.r.t.* matrix products in connection with its eigen-problem.
4. We experimentally verify the efficiency of our methods on real and synthetic data (Section 6). We find that P-Rank exponentially converges *w.r.t.* the iteration number. The stability of P-Rank is determined by the damping factors and weighting factors. The ASAP algorithm outperforms baseline algorithms on undirected graphs.

2 Preliminaries

In this section, we first give a brief overview of the P-Rank model. We then present notations and formulations of the P-Rank similarity.

2.1 An Overview of P-Rank

The basic essence of the P-Rank similarity model is distilled from the standard concept of SimRank metric [5]. Concretely, the theme of P-Rank involves three facets below:

1. Two distinct objects are similar if they are referenced by similar objects. (in-link recursion)
2. Two distinct objects are similar if they reference similar objects. (out-link recursion)
3. Every object is maximally similar to itself. (a base case)

Based on these facets, P-Rank scores, as described in its name, flowing from the incoming neighbors of objects are able to penetrate the outgoing neighbors. The concise elegance of the P-Rank intuition makes it one of the useful and cutting-edge structural metrics in the link-based analysis of information networks.

2.2 Notations

symbol	designation	symbol	designation
$\mathcal{G}$	information network	$s(a,b)$	P-Rank score between vertices a and b
$\mathcal{I}(a)$	in-neighbors of vertex a	C_{in} / C_{out}	in-link / out-link damping factor
$\mathcal{O}(a)$	out-neighbors of vertex a	λ	weighting factor
n	number of vertices in $\mathcal{G}$	$\mathbf{A}$	adjacency matrix of $\mathcal{G}$
m	number of edges in $\mathcal{G}$	$\mathbf{S}$	P-Rank similarity matrix of $\mathcal{G}$
K	number of iterations	$\mathbf{I}$	identity matrix

2.3 Formulation of P-Rank Model

We first define the network graph, and then introduce the P-Rank formulation.

Network Graph. A *network* is a labeled graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{A}; l)$, in which (i) $\mathcal{V}$ is a finite set of vertices. A partition of $\mathcal{V}$ is formed by dividing $\mathcal{V}$ into N disjointed domain-specific parts $\mathcal{V}_i$ $(i = 1, \cdots, N)$ *s.t.* $\mathcal{V} = \bigcup_{i=1}^{N} \mathcal{V}_i$ and $\mathcal{V}_i \cap \mathcal{V}_j = \varnothing$ if $i \neq j$; (ii) $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ is an edge set, and each vertex-pair $(u, v) \in \mathcal{E}$ denotes an edge from vertex u to v; (iii) $\mathcal{A}$ is a finite alphabet set, with a labeling function $l : \mathcal{V} \to \mathcal{A}$.

Based on the network graph, P-Rank model can be formulated as follows:

P-Rank Similarity. Given a network $\mathcal{G}$, for any two distinct vertices $u, v \in \mathcal{V}$, we define a scoring function $s(u, v) \in [0, 1]$ as follows:

$$s(u,u)=1; \tag{1}$$

$$s(u,v)=\underbrace{\frac{\lambda \cdot C_{\text{in}}}{|\mathcal{I}(u)|\,|\mathcal{I}(v)|}\sum_{i=1}^{|\mathcal{I}(u)|}\sum_{j=1}^{|\mathcal{I}(v)|} s\left(\mathcal{I}_i(u), \mathcal{I}_j(v)\right)}_{\text{in-link part}} + \underbrace{\frac{(1-\lambda)\cdot C_{\text{out}}}{|\mathcal{O}(u)|\,|\mathcal{O}(v)|}\sum_{i=1}^{|\mathcal{O}(u)|}\sum_{j=1}^{|\mathcal{O}(v)|} s\left(\mathcal{O}_i(u), \mathcal{O}_j(v)\right)}_{\text{out-link part}} \tag{2}$$

where (i) $\lambda \in [0, 1]$ balances the contributions of in- and out-links, (ii) C_{in} and $C_{\text{out}} \in (0, 1)$ are the damping factors for in- and out-link directions, respectively, (iii) $\mathcal{I}_i(u)$ and $\mathcal{O}_i(u)$ are the individual members of $\mathcal{I}(u)$ and $\mathcal{O}(u)$, respectively, and (iv) $|\mathcal{I}(u)|$ and $|\mathcal{O}(u)|$ are the cardinalities of $\mathcal{I}(u)$ and $\mathcal{O}(u)$, respectively.

It is worth noting that to avoid $s(u, v) = \infty$ when $|\mathcal{I}(\cdot)|$ or $|\mathcal{O}(\cdot)| = 0$, we define: (a) the in-link part of Eq.(2)$= 0$ if $\mathcal{I}(u) \cup \mathcal{I}(v) = \varnothing$; (b) the out-link part of Eq.(2)$= 0$ if $\mathcal{O}(u) \cup \mathcal{O}(v) = \varnothing$; (c) $s(u, v) = 0$, if $(\mathcal{I}(u) \cup \mathcal{I}(v)) \cap (\mathcal{O}(u) \cup \mathcal{O}(v)) = \varnothing$.

P-Rank Iterative Paradigm. To compute the P-Rank similarity $s(u, v)$ of Eq.(2), the conventional approach is to construct an iterative paradigm as follows:

$$s^{(0)}(u,v) = \begin{cases} 0, \text{ if } u \neq v; \\ 1, \text{ if } u = v. \end{cases} \tag{3}$$

For each $k = 0, 1, 2, \cdots$, the $(k+1)$-th iterate $s^{(k+1)}(\cdot,\cdot)$ can be computed as

$$\begin{aligned}
&s^{(k+1)}(u,u) = 1.\\
&s^{(k+1)}(u,v) = \frac{\lambda \cdot C_{\text{in}}}{|\mathcal{I}(u)||\mathcal{I}(v)|} \sum_{i=1}^{|\mathcal{I}(u)|}\sum_{j=1}^{|\mathcal{I}(v)|} s^{(k)}\left(\mathcal{I}_i(u), \mathcal{I}_j(v)\right)\\
&\qquad\qquad + \frac{(1-\lambda)\cdot C_{\text{out}}}{|\mathcal{O}(u)||\mathcal{O}(v)|} \sum_{i=1}^{|\mathcal{O}(u)|}\sum_{j=1}^{|\mathcal{O}(v)|} s^{(k)}\left(\mathcal{O}_i(u), \mathcal{O}_j(v)\right).\\
&s^{(k+1)}(u,v) = \text{the in-link part of Eq.(4), if } \mathcal{O}(u) \cup \mathcal{O}(v) = \varnothing,\\
&s^{(k+1)}(u,v) = \text{the out-link part of Eq.(4), if } \mathcal{I}(u) \cup \mathcal{I}(v) = \varnothing.
\end{aligned} \tag{4}$$

where $s^{(k)}(u,v)$ is the k-th iterative P-Rank score between vertices u and v. It has been proved in [7] that the exact similarity $s(u,v)$ is the supremum of $\{s^{(k)}(u,v)\}_{k=0}^{\infty}$, denoted by $\sup_k\{s^{(k)}(u,v)\}$, *i.e.,*

$$\lim_{k\to\infty} s^{(k)}(u,v) = \sup_{k\geq 0}\{s^{(k)}(u,v)\} = s(u,v) \quad (\forall u, v \in \mathcal{V}). \tag{5}$$

3 Accuracy Estimate on P-Rank Iteration

Based on Eq.(4), the iterative P-Rank similarity sequence $\{s^{(k)}(\cdot,\cdot)\}_{k=0}^{\infty}$ was known to converge monotonically [7]. However, the gap between the k-th iterative similarity $s^{(k)}(\cdot,\cdot)$ and the exact similarity $s(\cdot,\cdot)$ still remains unknown. Practically, quantifying this gap is very important in estimating the accuracy of iteratively computing P-Rank. For instance, given a tolerated error $\epsilon > 0$, one may naturally ask "What is the number of P-Rank iterations needed for achieving such an accuracy?".

This motivates us to study *the P-Rank accuracy estimate problem*. Given a network $\mathcal{G}$, for any iteration number $k = 1, 2, \cdots$, it is to find an upper bound ϵ_k of the gap between the k-th iterative similarity $s^{(k)}(\cdot,\cdot)$ and the exact $s(\cdot,\cdot)$, *s.t.* $|s^{(k)}(u,v) - s(u,v)| \leq \epsilon_k$ for any vertices u and v in $\mathcal{G}$.

The main result of this section is the following.

Theorem 1. *The P-Rank accuracy estimate problem has a tight upper bound*

$$\epsilon_k = (\lambda C_{in} + (1-\lambda)C_{out})^{k+1}$$

such that

$$|s^{(k)}(u,v) - s(u,v)| \leq \epsilon_k. \quad (\forall k = 0, 1, \cdots,\ \forall u, v \in \mathcal{V}) \tag{6}$$

A detailed proof of Theorem 1 can be found in [11] due to space limitations.

Theorem 1 provides an a-priori estimate for the gap between iterative and exact P-Rank similarity scores, which solely hinges on the weighing factor λ, the in- and out-link damping factors C_{in} and C_{out}, and the number k of iterations. To ensure more accurate P-Rank estimation results, it can be discerned from $\epsilon_k = (\lambda C_{\text{in}} + (1-\lambda)C_{\text{out}})^{k+1}$ $= (\lambda(C_{\text{in}} - C_{\text{out}}) + C_{\text{out}})^{k+1}$ that the smaller choices of C_{in} and C_{out} (i) with a smaller λ if $C_{\text{in}} > C_{\text{out}}$, or (ii) with a larger λ if $C_{\text{in}} < C_{\text{out}}$, are more preferable.

Example 1. Setting $C_{\text{in}} = 0.6, C_{\text{out}} = 0.4, \lambda = 0.3, k = 5$ will produce the following hight accuracy :

$$\epsilon_k = (0.3 \times 0.6 + (1-0.3) \times 0.4)^{5+1} = 0.0095. \qquad \square$$

Notice that the upper bound in Eq.(6) is attainable. Consider the network $\mathcal{G}_0$ depicted in Figure 1. It is apparent that $s^{(0)}(u,v) = 0$. For $k = 1, 2, \cdots$, it can be easily obtained that $s^{(k)}(u,v) = \lambda C_{\text{in}} + (1-\lambda)C_{\text{out}}$, which implies that $s(u,v) = \lambda C_{\text{in}} + (1-\lambda)C_{\text{out}}$. Hence, in the case of $k = 0$, $|s(u,v) - s^{(k)}(u,v)| = (\lambda C_{\text{in}} + (1-\lambda)C_{\text{out}})^{0+1}$ gives the precise upper bound in Eq.(6).

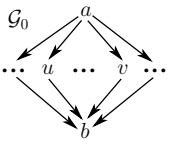


Fig. 1. "=" of Eq.(6) is attainable

Moreover, in the special case of $\lambda = 1$, Eq.(6) can be simplified to the SimRank accuracy estimate problem given in [8]. From this perspective, P-Rank accuracy estimate problem is the extension of Proposition 1 in [8] by jointly considering both in- and out-links of similarity computation.

Conversely, the exponential P-Rank convergence rate in Theorem 1 also implies that the number k of P-Rank iterations needed for attaining a desired accuracy ϵ amounts to

$$k = \lceil \log \epsilon / \log (\lambda \cdot C_{\text{in}} + (1-\lambda) \cdot C_{\text{out}}) \rceil .$$

4 Stability Analysis of P-Rank Model

In this section, we investigate the important issues of P-Rank sensitivity and stability. We first reformulate the P-Rank formulae in matrix notations (Subsect. 4.1). Using this representation, we then give a rigorous bound of the P-Rank conditional number for its stability analysis (Subsect. 4.2).

4.1 P-Rank Matrix Representation

We start by introducing the following symbols used throughout this section.

For a network $\mathcal{G}$ with n vertices, we denote by (i) $\mathbf{A} = (a_{i,j}) \in \mathbb{R}^{n \times n}$ the *adjacency matrix* of $\mathcal{G}$ whose entry $a_{i,j}$ equals 1, if there exists an edge from vertex i to j; or 0, otherwise, (ii) $\mathbf{S} = (s_{i,j}) \in \mathbb{R}^{n \times n}$ the *P-Rank similarity matrix* whose entry $s_{i,j}$ is equal to P-Rank score $s(i,j)$, and (iii) $\mathbf{Q} = (q_{i,j}) \in \mathbb{R}^{n \times n}$ and $\mathbf{P} = (p_{i,j}) \in \mathbb{R}^{n \times n}$ the *one-step backward and forward transition probability matrix* of $\mathcal{G}$, respectively, whose entries defined as follows:

$$q_{i,j} \triangleq \begin{cases} a_{j,i} / \sum_{j=1}^{n} a_{j,i}, & \text{if } \mathcal{I}(i) \neq \varnothing; \\ 0, & \text{if } \mathcal{I}(i) = \varnothing. \end{cases} \qquad p_{i,j} \triangleq \begin{cases} a_{i,j} / \sum_{j=1}^{n} a_{i,j}, & \text{if } \mathcal{O}(i) \neq \varnothing; \\ 0, & \text{if } \mathcal{O}(i) = \varnothing. \end{cases} \tag{7}$$

With the above notations, the P-Rank formulae (1) and (2) can be rewritten as[1]

$$\mathbf{S} = \lambda C_{\text{in}} \cdot \mathbf{Q} \cdot \mathbf{S} \cdot \mathbf{Q}^T + (1-\lambda) C_{\text{out}} \cdot \mathbf{P} \cdot \mathbf{S} \cdot \mathbf{P}^T + (1 - \lambda C_{\text{in}} - (1-\lambda) C_{\text{out}}) \cdot \mathbf{I}_n, \tag{8}$$

Also, dividing both sides of Eq.(8) by $(1 - \lambda C_{\text{in}} - (1-\lambda)C_{\text{out}})$ results in

$$\mathbf{S}' = \lambda C_{\text{in}} \cdot \mathbf{Q} \cdot \mathbf{S}' \cdot \mathbf{Q}^T + (1-\lambda) C_{\text{out}} \cdot \mathbf{P} \cdot \mathbf{S}' \cdot \mathbf{P}^T + \mathbf{I}_n, \text{ and} \tag{9}$$

[1] Although in this case the diagonal entries of $\mathbf{S}$ are not equal to 1, $\mathbf{S}$ still remains diagonally dominant, which ensures that "every vertex is maximally similar to itself". Li *et al.* [12] has showed that this revision for SimRank matrix representation is reasonable, which can be applied in the similar way to P-Rank.

$$\mathbf{S} = (1 - \lambda C_{\text{in}} - (1-\lambda)C_{\text{out}}) \cdot \mathbf{S}'.$$

Comparing Eq.(8) with Eq.(9), we see that the coefficient $(1 - \lambda C_{\text{in}} - (1-\lambda)C_{\text{out}})$ of $\mathbf{I}_n$ in Eq.(8) merely contributes an overall multiplicative factor to P-Rank similarity. Hence, setting the coefficient to 1 in Eq.(8) still preserves the *relative* magnitude of the P-Rank score though the diagonal entries of $\mathbf{S}$ in this scenario might not equal 1[2].

4.2 Conditional Number of P-Rank

Using the P-Rank matrix model of Eq.(9), we next theoretically analyze the stability of P-Rank, by determining its *conditional number* $\kappa_\infty(\cdot)$ in the infinity norm sense, which has important implications for the sensitivity of P-Rank computation. One complicated factor in P-Rank stability analyses is to bound the conditional number $\kappa_\infty(\cdot)$.

Before giving a formal definition of $\kappa_\infty(\cdot)$, we first introduce the following notations: (i) We denote by $\text{vec}(\mathbf{X}) \in \mathbb{R}^{n^2}$ the *vectorization* of the matrix $\mathbf{X} \in \mathbb{R}^{n \times n}$ formed by stacking the columns of $\mathbf{X}$ into a single column vector, and (ii) the operator $\otimes$ the *Kronecker product* of two matrices.

Taking $\text{vec}(\cdot)$ on both sides of Eq.(9) and applying the Kronecker property of $(\mathbf{B}^T \otimes \mathbf{A})\text{vec}(\mathbf{X}) = \text{vec}(\mathbf{AXB})$ [13], we have

$$\text{vec}(\mathbf{S}) = \lambda C_{\text{in}}(\mathbf{Q} \otimes \mathbf{Q})\text{vec}(\mathbf{S}) + (1-\lambda)C_{\text{out}}(\mathbf{P} \otimes \mathbf{P})\text{vec}(\mathbf{S}) + \text{vec}(\mathbf{I}_n).$$

Rearranging terms in the above equation produces

$$\underbrace{(\mathbf{I}_{n^2} - \lambda C_{\text{in}}(\mathbf{Q} \otimes \mathbf{Q}) - (1-\lambda)C_{\text{out}}(\mathbf{P} \otimes \mathbf{P}))}_{\triangleq \mathbf{M}} \cdot \underbrace{\text{vec}(\mathbf{S})}_{\triangleq \mathbf{s}} = \underbrace{\text{vec}(\mathbf{I}_n)}_{\triangleq \mathbf{b}}. \tag{10}$$

Notice that Eq.(10) is a *linear* system of n^2 equations in terms of $s_{i,j}$ in nature as it can be reduced in the form of $\mathbf{M} \cdot \mathbf{s} = \mathbf{b}$, as illustrated in Eq.(10).

Based on Eq.(10), we now give a formal definition of *P-Rank conditional number*.

Definition 1 (P-Rank conditional number). *For a network $\mathcal{G}$, let $\mathbf{Q}$ and $\mathbf{P}$ be the one-step backward and forward transition probability matrix of $\mathcal{G}$, respectively, defined by Eq.*(7)*, and let*

$$\mathbf{M} \triangleq \mathbf{I}_{n^2} - \lambda C_{in}(\mathbf{Q} \otimes \mathbf{Q}) - (1-\lambda)C_{out}(\mathbf{P} \otimes \mathbf{P}). \tag{11}$$

The P-Rank conditional number of $\mathcal{G}$, denoted by $\kappa_\infty(\mathcal{G})$, is defined as

$$\kappa_\infty(\mathcal{G}) \triangleq \|\mathbf{M}\|_\infty \cdot \|\mathbf{M}^{-1}\|_\infty, \tag{12}$$

where $\|\cdot\|_\infty$ is the ∞-norm that returns the maximum absolute row sum of the matrix.

The conditional number is introduced for being applied to P-Rank stability analysis.

Theorem 2. *Given the network $\mathcal{G}$, for any weighting factor $\lambda \in [0,1]$ and in- and out-link damping factors $C_{in}, C_{out} \in (0,1)$, the P-Rank problem has the following tight bound of conditional number*

$$\kappa_\infty(\mathcal{G}) \leq \frac{1 + \lambda \cdot C_{in} + (1-\lambda) \cdot C_{out}}{1 - \lambda \cdot C_{in} - (1-\lambda) \cdot C_{out}}. \tag{13}$$

[2] In what follows, we shall base our techniques on the P-Rank matrix form of Eq.(9).

For the interest of space, please refer to [11] for a detailed proof of Theorem 2.

Theorem 2 provides a tight upper bound of the P-Rank conditional number $\kappa_\infty(\mathcal{G})$. Intuitively, the value of $\kappa_\infty(\mathcal{G})$ measures how stable the P-Rank similarity score is to the changes either in the link structure of the network $\mathcal{G}$ (by inserting or deleting vertices or edges), or in the damping and weighting factors of $C_{\text{in}}, C_{\text{out}}$ and λ.

To get a feel for how $\kappa_\infty(\mathcal{G})$ affects P-Rank sensitivity, we denote by $\Delta\mathbf{A}$ the updates in $\mathcal{G}$ to the adjacency matrix $\mathbf{A}$, $\Delta\mathbf{M}$ (*resp.* $\Delta\mathbf{s}$) the changes (caused by $\Delta\mathbf{A}$) to $\mathbf{M}$ (*resp.* $\mathbf{s}$) defined in Eq.(10). As Eq.(10) is a linear equation, it is known that

$$\frac{\|\Delta\mathbf{s}\|_\infty}{\|\mathbf{s}\|_\infty} \leq \kappa_\infty(\mathcal{G}) \cdot \frac{\|\Delta\mathbf{M}\|_\infty}{\|\mathbf{M}\|_\infty} \leq \frac{1+\lambda\cdot C_{\text{in}}+(1-\lambda)\cdot C_{\text{out}}}{1-\lambda\cdot C_{\text{in}}-(1-\lambda)\cdot C_{\text{out}}} \cdot \frac{\|\Delta\mathbf{M}\|_\infty}{\|\mathbf{M}\|_\infty}. \tag{14}$$

This tells that the small $\kappa_\infty(\mathcal{G})$ (*i.e.,* small choices for C_{in} and C_{out}) would make P-Rank stable, implying that a small change $\Delta\mathbf{M}$ in the link structure to $\mathbf{M}$ may not cause a large change $\Delta\mathbf{s}$ in P-Rank scores. Conversely, the large value of $\kappa_\infty(\mathcal{G})$ would make P-Rank *ill-conditioned*.

To see how the weighting factor λ affects $\kappa_\infty(\mathcal{G})$, we compute the partial derivatives of the bound for $\kappa_\infty(\mathcal{G})$ *w.r.t.* λ to get

$$\frac{\partial}{\partial\lambda}\left(\frac{1+\lambda\cdot C_{\text{in}}+(1-\lambda)\cdot C_{\text{out}}}{1-\lambda\cdot C_{\text{in}}-(1-\lambda)\cdot C_{\text{out}}}\right) = \frac{2\,(C_{\text{in}}-C_{\text{out}})}{(1-\lambda\cdot C_{\text{in}}-(1-\lambda)\cdot C_{\text{out}})^2}, \tag{15}$$

which implies that when $C_{\text{in}} > C_{\text{out}}$ (*resp.* $C_{\text{in}} < C_{\text{out}}$), for the increasing λ, a small change in $\mathcal{G}$ may result in a large (*resp.* small) change in P-Rank, which makes P-Rank an *ill-conditioned* (*resp. a well-conditioned*) problem; when $C_{\text{in}} = C_{\text{out}}$, the value of $\kappa_\infty(\mathcal{G})$ is independent of λ.

5 An Efficient Algorithm for P-Rank Estimating on Undirected Graphs

In this section, we study the P-Rank optimization problem over undirected networks.

The key idea in our optimization is to maximally use the adjacency matrix $\mathbf{A}$ to characterize the P-Rank similarity $\mathbf{S}$ as a power series in a function form like $\mathbf{S} = \sum_{k=0}^{+\infty} f(\mathbf{A}^k)$. The rationale behind this is that $\mathbf{A} = \mathbf{A}^T$ for undirected networks, implying that there exists a diagonal matrix $\mathbf{D}$ such that $\mathbf{Q} = \mathbf{P} = \mathbf{D}\cdot\mathbf{A}$ in Eq.(8). Hence, computing $\mathbf{S}$ boils down to solving $\sum_{k=0}^{+\infty} f(\mathbf{A}^k)$. For computing $f(\mathbf{A}^k)$, it is far less costly to first diagonalize $\mathbf{A}$ into $\mathbf{\Lambda}$ via eigen-decomposition than to compute $\mathbf{A}^k$ in a brute-force way. Then calculating $f(\mathbf{A}^k)$ reduces to computing the function on each eigenvalue for $\mathbf{A}$.

More specifically, the main result of this section is the following.

Theorem 3. *For undirected networks, the P-Rank similarity problem of Eq.*(8) *can be solvable in* $O(n^3)$ *worst-case time.*

It is worth noting that SimRank over undirected graphs is a special case of the more general P-Rank when $\lambda = 1$ and $C_{\text{in}} = C_{\text{out}}$. In contrast to the $O(n^3 + Kn^2)$-time of

Algorithm 1. ASAP $(\mathcal{G}, \lambda, C_{\text{in}}, C_{\text{out}})$

Input : a labeled undirected network $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{A}; l)$, the weighting factor λ, and in- and out-link damping factors C_{in} and C_{out}.

Output: similarity matrix $\mathbf{S} = (s_{i,j})_{n\times n}$ with $s_{i,j}$ denoting P-Rank score between vertices i and j.

1 initialize the adjacency matrix $\mathbf{A}$ of $\mathcal{G}$;

2 compute the diagonal matrix $\mathbf{D} = diag(d_{1,1}, d_{2,2}, \cdots, d_{n,n})$ with its entry $d_{i,i} = (\sum_{j=1}^{n} a_{i,j})^{-1}$, if $\sum_{j=1}^{n} a_{i,j} \neq 0$; and $d_{i,i} = 0$, otherwise;

3 compute the auxiliary matrix $\mathbf{T} = \mathbf{D}^{1/2} \cdot \mathbf{A} \cdot \mathbf{D}^{1/2}$

4 decompose $\mathbf{T}$ into the diagonal matrix $\mathbf{\Lambda} = diag(\Lambda_{1,1}, \Lambda_{2,2}, \cdots, \Lambda_{n,n})$ and the orthogonal $\mathbf{U}$ via QR factorization *s.t.* $\mathbf{T} = \mathbf{U} \cdot \mathbf{\Lambda} \cdot \mathbf{U}^T$;

5 compute the auxiliary matrix $\mathbf{\Gamma} = (\Gamma_{i,j})_{n\times n} = \mathbf{U}^T \cdot \mathbf{D}^{-1} \cdot \mathbf{U}$ and $\mathbf{V} = \mathbf{D}^{1/2} \cdot \mathbf{U}$ and the constant $C = \lambda C_{\text{in}} + (1-\lambda) C_{\text{out}}$;

6 compute the matrix $\mathbf{\Psi} = (\psi_{i,j})_{n\times n}$ whose entry $\psi_{i,j} = \Gamma_{i,j}/(1 - C \cdot \Lambda_{i,i} \cdot \Lambda_{j,j})$;

7 compute the P-Rank similarity matrix $\mathbf{S} = (1-C) \cdot \mathbf{V} \cdot \mathbf{\Psi} \cdot \mathbf{V}^T$;

8 **return** $\mathbf{S}$;

SimRank optimization over undirected graphs in our early work [14], this work further optimizes P-Rank time in $O(n^3)$ with no need for iteration.

To show Theorem 3, we first characterize P-Rank elegantly on undirected graphs.

Theorem 4. *For the undirected network $\mathcal{G}$ with n vertices, let (i) $\mathbf{A} = (a_{i,j}) \in \mathbb{R}^{n\times n}$ be the adjacency matrix of $\mathcal{G}$, (ii) $\mathbf{D} \in \mathbb{R}^{n\times n}$ is a diagonal matrix*[3]*.*

$$\mathbf{D} = diag((\sum_{j=1}^{n} a_{1,j})^{-1}, \cdots, (\sum_{j=1}^{n} a_{n,j})^{-1}), \tag{16}$$

and (iii) $\mathbf{U}$ and $\mathbf{\Lambda}$ the eigen-decomposition results of the matrix $\mathbf{D}^{1/2}\mathbf{A}\mathbf{D}^{1/2}$, in which $\mathbf{U} \in \mathbb{R}^{n\times n}$ is an orthogonal matrix whose columns are all eigenvectors of $\mathbf{D}^{1/2}\mathbf{A}\mathbf{D}^{1/2}$, and $\mathbf{\Lambda} = (\Lambda_{i,j}) \in \mathbb{R}^{n\times n}$ is an diagonal matrix with its diagonal entries being all eigenvalues of $\mathbf{D}^{1/2}\mathbf{A}\mathbf{D}^{1/2}$.

Then the P-Rank similarity matrix $\mathbf{S}'$ of Eq.(9) *can be explicitly computed as*[4]*.*

$$\mathbf{S}' = \mathbf{D}^{1/2}\mathbf{U} \cdot \mathbf{\Psi} \cdot \mathbf{U}^T\mathbf{D}^{1/2}, \tag{17}$$

where

$$\mathbf{\Psi} = (\Psi_{i,j})_{n\times n} = \left(\frac{[\mathbf{U}^T\mathbf{D}^{-1}\mathbf{U}]_{i,j}}{1 - (\lambda \cdot C_{in} + (1-\lambda) \cdot C_{out})\, \Lambda_{i,i}\Lambda_{j,j}} \right)_{n\times n}, \text{ and} \tag{18}$$

$[\mathbf{U}^T\mathbf{D}^{-1}\mathbf{U}]_{i,j}$ *denotes the (i,j)-entry of the matrix $\mathbf{U}^T\mathbf{D}^{-1}\mathbf{U}$.*

Due to space limitations, a detailed proof of this theorem can be found in [11].

We next prove Theorem 3 by providing an algorithm for P-Rank computation over undirected networks.

[3] We define $\frac{1}{0} \triangleq 0$, thereby avoiding division by zero when the column/row sum of $\mathbf{A}$ equals 0.

[4] $\mathbf{D}^{1/2}$ is a diagonal matrix whose diagonal entries are the principal square root of those of $\mathbf{D}$.

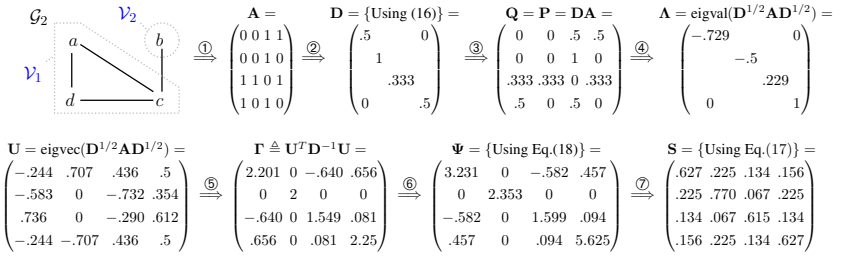


Fig. 2. An example of computing P-Rank over undirected network $\mathcal{G}_2$ via non-iterative method

Algorithm. The algorithm, referred to as ASAP , is shown in Algorithm 1. It takes as input a labeled undirected network $\mathcal{G}$, a weighting factor λ, and in- and out-link damping factors C_{in} and C_{out}; and it returns the P-Rank similarity matrix $\mathbf{S}=(s_{i,j})_{n\times n}$ of all vertex-pairs in $\mathcal{G}$.

The algorithm ASAP works as follows. It first initializes the adjacency matrix $\mathbf{A}$ of the network $\mathcal{G}$ (line 1). Using $\mathbf{A}$, it then compute the auxiliary diagonal matrix $\mathbf{D}$ whose (i,i)-entry equals the reciprocal of the i-th column sum of $\mathbf{A}$, if this reciprocal exists; or 0, otherwise (line 1). ASAP then uses QR eigen-decomposition [13] to factorize $\mathbf{D}^{1/2}\mathbf{A}\mathbf{D}^{1/2}$ as $\mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$, in which all columns of $\mathbf{U}$ are the eigenvectors of $\mathbf{D}^{1/2}\mathbf{A}\mathbf{D}^{1/2}$, and all diagonal entries of $\mathbf{\Lambda}$ are the corresponding eigenvalues of $\mathbf{D}^{1/2}\mathbf{A}\mathbf{D}^{1/2}$ (lines 1-1). Utilizing $\mathbf{U}$ and $\mathbf{\Lambda}$, it calculates $\mathbf{\Psi}$ (lines 1-1) to obtain the similarity matrix $\mathbf{S}$ (lines 1-1), which can be justified by Eqs.(17) and (18).

We now give a running example to show how ASAP computes the P-Rank similarity matrix $\mathbf{S}$ for a given network.

Example 2. Consider a labeled undirected network $\mathcal{G}_2$ with 4 vertices $\mathcal{V}=\mathcal{V}_1\cup\mathcal{V}_2=\{a,c,d\}\cup\{b\}$ and 4 edges $\mathcal{E}=\{(a,c),(a,d),(c,d),(b,c)\}$. Figure 2 depicts the detailed process of computing $\mathbf{S}$ step by step with no need for any iteration. ASAP returns $\mathbf{S}$ as the P-Rank matrix, which is exactly the solution to the P-Rank formula of Eq.(8).

To complete the proof of Theorem 3, we next show that algorithm ASAP has cubic-time complexity bound in the number of vertices.

Complexity. (i) In lines 1-1, computing the diagonal $\mathbf{D}$ and $\mathbf{T}=\mathbf{D}^{1/2}\mathbf{A}\mathbf{D}^{1/2}$ takes $O(m)$ and $O(n^2)$ time, respectively, with n and m being the number of vertices and edges in $\mathcal{G}$ respectively. (ii) In line 1, QR factorization of $\mathbf{T}$ into the orthogonal $\mathbf{U}$ and the diagonal $\mathbf{\Lambda}$ requires $O(n^3)$ worse-case time. (iii) In lines 1-1, computing the auxiliary matrices $\mathbf{\Gamma}$, $\mathbf{V}$, $\mathbf{\Psi}$ and the similarity matrix $\mathbf{S}$ yields $O(n^3), O(n^2), O(n^2)$ and $O(n^3)$, respectively, which can be bounded by $O(n^3)$. Combining (i), (ii) and (iii), the total time of ASAP is in $O(n^3)$.

6 Experimental Evaluation

We next present an experimental study of our P-Rank estimating methods. Using real-life and synthetic data, we conducted two sets of experiments to evaluate the accuracy, stability, computational efficiency of our approaches for similarity estimation *v.s.* (a)

the conventional pruning P-Rank iterative paradigm [7] and (b) the memoization-based P-Rank algorithm [8,7].

Experimental setting. We used real-life data and synthetic data.

(1) Real-life data. The real-life data was taken from DBLP [5]. We extracted the 10-year (from 1998 to 2007) author-paper information from the entire DBLP dataset. We picked up papers published on 6 major conferences ("ICDE", "VLDB", "SIGMOD","WWW", "SIGIR" and "KDD"). Every two years made a time step. For each time step, we built a co-authorship network incrementally from the one of previous time step. We chose the relationship that there is an edge between authors if one author wrote a paper with another. The sizes of these DBLP networks are as follows:

DBLP Data	1998-1999	1998-2001	1998-2003	1998-2005	1998-2007
n	1,525	3,208	5,307	7,984	10,682
m	5,929	13,441	24,762	39,399	54,844

(2) Synthetic data. We also used a C++ boost generator to produce graphs, controlled by two parameters: the number n of vertices, and the number m of edges. We then produced a set of 5 networks (undirected RAND data) by increasing the vertex size n from 100K to 1M with edges randomly chosen.

(3) Algorithms. We have implemented the following algorithms in C++: (a) our algorithm ASAP ; (b) the conventional P-Rank iterative algorithm Iter [7] with the radius-based pruning technique; (c) the memoization-based algorithm Memo [8] applied on P-Rank; (d) SimRank optimized algorithm AUG [14] over undirected graphs.

The experiments were run on a machine with a Pentium(R) Dual-Core (2.0GHz) CPU and 4GB RAM, using Windows Vista. Each experiment was repeated 5 times and the average is reported here.

For ease and fairness of comparison, the following parameters were used as default values (unless otherwise specified). We set the in-link damping factor $C_{\text{in}} = 0.8$, the out-link damping factor $C_{\text{out}} = 0.6$, the weighting factor $\lambda = 0.5$, the total iteration number $k = 10$, the desired accuracy $\epsilon = 0.001$.

Experimental Results. We now present our findings.

Exp-1: Accuracy. In the first set of experiments, we evaluated the accuracy of P-Rank iteration in Eq.(6) using synthetic and real data. We also investigated the impact of in- and out-link damping factors on P-Rank accuracy, using synthetic data.

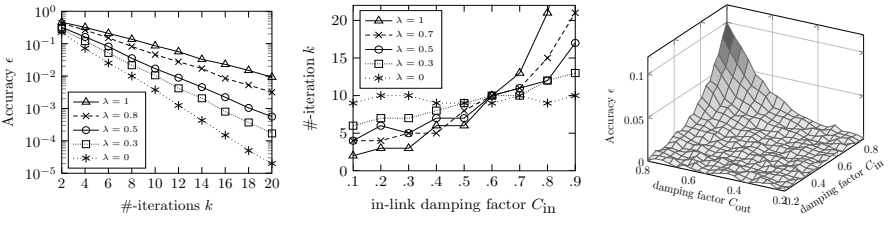
We considered various weighting factors λ from 0 to 1 for 5 RAND networks. For each RAND data with vertex size ranged from 0.2M to 1M, fixing the damping factors $C_{\text{in}} = 0.8$ and $C_{\text{out}} = 0.6$, we varied the number k of P-Rank iterations in Eq.(4) ranged from 2 to 20 for each vertex-pair. Due to space limitations, Figure 3(a) only reports the results over the RAND network (with 1M vertices), which visualizes the P-Rank accuracy *w.r.t.* the number of iterations performed. Here, the accuracy is measured

[5] http://www.informatik.uni-trier.de/~ley/db/

by the absolute difference between the iterative P-Rank and the exact solution[6]. Note that the logarithmic scale is chosen across the y-axis in Figure 3(a) to provide a more illustrative look for the asymptotic rate of P-Rank convergence. For each fixed λ, the downward lines for P-Rank iterations reveal an exponential accuracy as k increases, as expected in Theorem 1. We also observe that the larger λ may dramatically increase the slope of a line, which tells that increasing the weighting factor decreases the rate of convergence for P-Rank iteration.

Using the same RAND , we fixed the desired accuracy $\epsilon = 0.001$ and varied damping factors by increasing C_{in} and C_{out} from 0.1 to 0.9. Fixing $C_{\text{out}} = 0.6$, the result of varying C_{in} is reported in Figure 3(b) (for space constraints, a similar result of varying C_{out} is omitted), in which the x-axis represents the value of in-link damping factor, and y-axis gives the number of iterations needed for attaining the given accuracy ϵ. When $\lambda = 0$, the curve in Figure (b) visually approaches a horizontal line. This is because in this case, P-Rank boils down to an iterative form of the reversed SimRank with no in-link similarity considered, which makes C_{in} insensitive to the final P-Rank score. When $0 < \lambda \leq 1$, k shows a general increased tendency as C_{in} is growing. This tells us that small choices of damping factors may reduce the number of iterations required for a fixed accuracy, and hence, improves the efficiency of P-Rank, as expected.

To evaluate the impact of both C_{in} and C_{out} *w.r.t.* the accuracy, we used the real DBLP data. We only report the result on DBLP 1998-2007 data in Figure 3(c), which shows a 3D shaded surface from the average of accuracy value for all vertex-pairs on z-axis when we fixed $k = 10$ and $\lambda = 0.5$, and varied C_{in} and C_{out} in x-axis and y-axis, respectively. It can be seen that the residual becomes huge only when C_{in} and C_{out} are both increasing to 1; and the iterative P-Rank is accurate when C_{in} and $C_{\text{out}} < 0.6$. This explains why small choices of damping factors are suggested in P-Rank iteration.



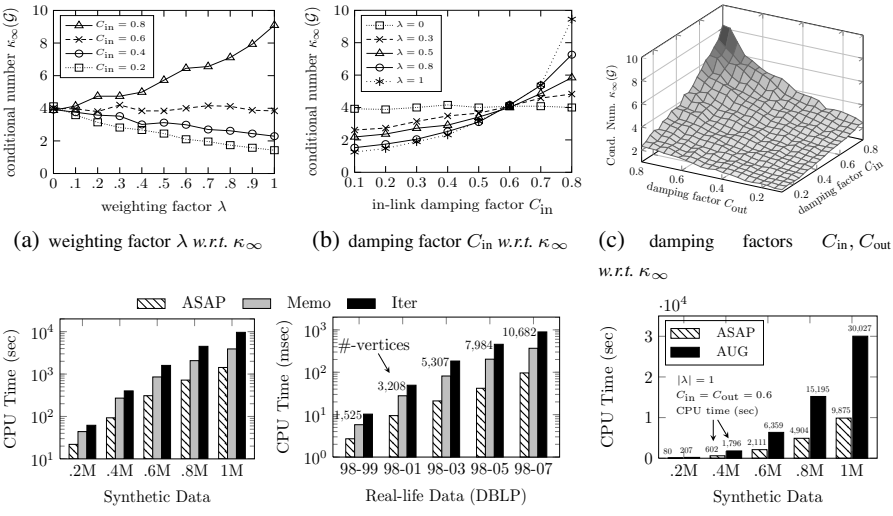
(a) #-iteration k *w.r.t.* accuracy ϵ (b) damping factor C_{in} *w.r.t.* k (c) damping factors $C_{\text{in}}, C_{\text{out}}$ *w.r.t.* ϵ

Fig. 3. Experimental Results on P-Rank Accuracy

Exp-2: Stability. We evaluated P-Rank stability using synthetic data and DBLP .

Fixing the value of out-link damping factor $C_{\text{out}} = 0.6$, we varied the values of C_{in} from 0.2 to 0.8. The result over RAND 1M data is reported in Figure 4(a), in which x-axis indicates various weighting factors λ with their sizes ranged from 0 to 1. Accordingly, varying λ from 0 and 1, Figure 4(b) visualizes the impact of in-link damping factor C_{in} on P-Rank stability when $C_{\text{out}} = 0.6$ is fixed.

[6] To select the P-Rank "exact" solution $s(\cdot,\cdot)$, we used *the Cauchy's criterion for convergence* and regarded the 100th iterative $s^{(100)}(\cdot,\cdot)$ score as the "exact" one *s.t.* $|s^{(100)}(\cdot,\cdot) - s^{(101)}(\cdot,\cdot)| \ll 1 \times 10^{-10}$.



(a) weighting factor λ *w.r.t.* κ_∞ (b) damping factor C_{in} *w.r.t.* κ_∞ (c) damping factors $C_{\text{in}}, C_{\text{out}}$ *w.r.t.* κ_∞

(d) #-vertices n *w.r.t.* CPU time over synthetic and real-life data (e) ASAP *v.s.* AUG on synthetic data

Fig. 4. Experimental Results on P-Rank Stability and Time Efficiency

The results in Figures 4(a) and 4(b) both show that increasing weighting factor λ induces a large P-Rank conditional number when $C_{\text{in}} > 0.6$. Notice that for different C_{in}, there is one common point $(\lambda, \kappa_\infty) = (0, 4)$ of intersection of all curves in Figure 4(a); correspondingly, in the extreme case of $\lambda = 0$, the curve in Figure 4(b) approaches to a horizontal line. These indicate that varying C_{in} when $\lambda = 0$ has no effect on the stability κ_∞ of P-Rank, for in this case only the contribution of out-links is considered for computing P-Rank similarity. When $C_{\text{in}} < 0.6$, however, $\kappa_\infty(\mathcal{G})$ is decreased as λ grows. This tells that small quantities of weighting factor and damping factors yield small P-Rank conditional numbers, and thus make the P-Rank well-conditioned, as expected in Theorem 2.

For real-life datasets, Figure 4(c) comprehensively depicts in 3D view the impacts of both C_{in} and C_{out} on P-Rank stability over DBLP 1M data, in which x- and y-axis represent in- and out-link damping factors respectively, and z-axis stands for the P-Rank conditional number. The result demonstrates that P-Rank is comparatively stable when both C_{in} and C_{out} are small (less than 0.6). However, when C_{in} and C_{out} are approaching to 1, P-Rank is ill-conditioned and not very useful since small perturbations in similarity computation may cause P-Rank scores drastically altered, which carries the risk of producing nonsensical similarity results. In light of this, small choices of damping factors are preferable.

Exp-3: Time Efficiency over Undirected Networks. In the third set of experiments, we used synthetic RAND and the real DBLP data to evaluate the benefits of the time-efficient algorithm ASAP . Figure 4(d) compares the performance of ASAP with those of Memo and Iter on both datasets. We use the logarithmic scale on the CPU time (y-axis). The iteration number for Iter and Memo is set to 10. Note that different time unit is chosen across the vertical axis in the two plots of Fig.4(d) to provide a clear

look for each bar shape. (i) Varying the number of vertices from 200K to 1M, the result on RAND indicates that ASAP outperformed Memo and Iter ; the computational time of ASAP has almost one order of magnitude faster than Iter , *i.e.,* computing P-Rank similarity from the explicit characterization of its solution is efficient. In most cases, there are a considerable amount of repeated iterations for Iter and Memo to reach a fixed-point of P-Rank scores, and these impede their time efficiency in P-Rank computation. (ii) The result on DBLP also shows the running time with respect to the number of nodes for P-Rank estimation when the sizes of DBLP data increased from 1.5K to 10K. In all cases, ASAP performed the best, by taking advantage of its non-iterative paradigm.

To compare the performances of ASAP and AUG , we applied them to compute SimRank similarities over synthetic RAND data, by setting $\lambda = 1$ for ASAP (a special case of P-Rank without out-links consideration). Figure 4(e) reports the result over synthetic RAND data. It can be seen that ASAP runs approx. 3 times faster than AUG though the CPU time of the ASAP and AUG are of the same order of magnitude. The reason is that after eigen-decomposition, AUG still requires extra iterations to be performed in the small eigen-subspace, which takes a significant amount of time, whereas ASAP can straightforwardly compute similarities in terms of eigenvectors with no need for iterations.

7 Related Work

There has been a surge of studies (*e.g.,* [2,15,3,9,4,5,16,6]) on link-based analysis over information networks in recent years. PageRank became popular since the famous result of Page *et al.* [6] was used by the Google search engine for ranking web sites based on link structures. Since then, a host of new ranking algorithms for web pages have been developed. The famous results include the HITS algorithm [2] proposed by Jon *et al.* (now used `www.ask.com`), SimRank [17,10,5], SimFusion [15,4] and P-Rank algorithm [7].

SimRank [5] is a recursive structural similarity measure based on the intuition that "*two objects are similar if they are related to similar objects* ", which extends the Bibliometric Coupling and Co-citation [3,1] beyond the local neighborhood so that the information of the entire network can be exploited globally. A naive iterative approach was initially proposed in [5] to compute the SimRank score with a pruning mechanism, which is in quartic worst-case time. Several optimization problems were investigated for SimRank estimation, including the pair-wise iterative methods [5,8], matrix-based approaches [8,12,17,14] and probabilistic algorithms [18].

More recently, Zhao *et al.* [7] presented a new P-Rank model when noticing the limited information problem of SimRank —the similarity scores are only determined by their in-link relationships. P-Rank measure refines SimRank by jointly considering both in- and out-links of entity pairs. The conventional algorithm for computing P-Rank is based on iterative techniques, which still requires quartic time complexity. To optimize its computational time, a similar memoization approach in [8] can be applied to P-Rank, which reduces its time to be cubic in the worst case. In comparison, our work focuses on the problems of P-Rank accuracy, stability and computational time over undirected graphs.

Closer to this work are [14,8]. A time-efficient algorithm AUG for SimRank computation was proposed on undirected graphs in [14], which is in $O(n^3 + kn^2)$ time. In contrast, we further improve [14] (i) by providing a non-iterative $O(n^3)$-time algorithm that explicitly characterizes the similarity solution, and (ii) by extending SimRank to the general P-Rank measure. An accuracy estimation for SimRank was addressed in [8], it differs from this work in that our focus is on P-Rank estimation, in which the accuracy depends on both in- and out-link damping factors rather than the in-link damping factor alone.

8 Conclusions

In this study, several P-Rank problems were investigated. First, we have proposed an accuracy estimate for the P-Rank iteration, by finding out the exact number of iterations needed to attain a given accuracy. Second, we have introduced the notion of P-Rank conditional number based on the matrix representation of P-Rank. A tight bound of P-Rank conditional number has been provided to show how the weighting factor and the damping factors affect the stability of P-Rank. Finally, we have also devised an $O(n^3)$-time algorithm to deal with the P-Rank optimization problem over undirected networks. Our empirical results have verified the accuracy, stability and computational efficiency of our approaches.

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