SimTab: Accuracy-Guaranteed SimRank Queries through Tighter Confidence Bounds and Multi-Armed Bandits

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ABSTRACT

SimRank is a classic measure of vertex-pair similarity according to the structure of graphs. Top-k and thresholding SimRank queries are two important types of similarity search with numerous applications in web mining, social network analysis, spam detection, etc. However, extensive studies for SimRank most focus on single-pair and single-source queries and fail to provide any feasible solution for the top-k and thresholding queries, e.g., with theoretical accuracy guarantee or acceptable empirical performance. In this paper, we propose *SimTab* (SimRank queries with Tighter confidence bounds and multi-armed bandits) to answer top-k and thresholding queries in a unified manner. First, we integrate several techniques with random walk sampling to tighten the confidence bound of SimRank estimation, which enhances the query efficiency. Second, we answer top-k and thresholding queries from the perspective of the Multi-Armed Bandits (MAB) problems. The proposed algorithms significantly improve the theoretical efficiency over state of the art, whereas the algorithm complexity closely matches the hardness of the problem. We further propose a novel sampling strategy specially tailored for node similarity queries, which improves both the theoretical and practical query efficiency of the MAB-based algorithms. Our method is the first with query accuracy guarantee for these two queries, and the sole algorithm to achieve high-quality query results on large graphs. Moreover, all proposed algorithms are index-free, and thus can be naturally applied to dynamic graphs.

Extensive experiments on several large graph datasets demonstrate that our algorithms achieve much superior effectiveness with comparable or less query time cost than all index-free and index-based state of the art. Besides, our work proposes the first thorough empirical evaluation of the existing SimRank algorithms over top-k and thresholding queries.

1. INTRODUCTION

SimRank [16] is a widely adopted measure of the similarities of graph nodes, with numerous applications such as web mining [18], social network analysis [23], and spam detection [29]. The formulation of SimRank is based on a recursive concept, i.e., two objects are similar if they are linked to similar objects, while an object is most similar to itself. Given a graph $G = (V, E)$, the SimRank similarity between two nodes u and v is defined as:

$$s(u,v) = \begin{cases} 1, & \text{if } u = v \\ \dfrac{c}{|I(u)| \cdot |I(v)|} \displaystyle\sum_{x \in I(u)} \sum_{y \in I(v)} s(x,y), & \text{otherwise} \end{cases} \tag{1}$$

where $I(u)$ denotes the set of in-neighbors of u, and $c \in (0, 1)$ is a decay factor typically set to 0.6 or 0.8 [16, 25].

A plethora of techniques has been proposed for the efficient computation of SimRank. Since computing all-pair SimRank incurs excessive time and space cost for large-sized graphs, most existing work focuses on the single-pair and single-source queries[1]. The single-pair query answers the SimRank similarity of a given node pair (u, v), whereas the single-source query takes a query node u as input and returns the similarity of each node w.r.t. u. Due to the recursive definition of SimRank, its exact values can not be computed in limited time. Given an error parameter ε and a failure probability δ, we say the query result achieves *absolute error guarantee* [24, 30, 32], if with at least $1 - \delta$ probability, each returned estimated SimRank value $\hat{s}(u, v)$ satisfies that $|\hat{s}(u, v) - s(u, v)| \leq \varepsilon$.

Motivated by the real-world application scenarios [18, 23, 29], in this paper, we study the following top-k and thresholding queries.

Definition 1 (Top-k Query). *We are given a node u in G, a positive integer $k < n$, and a failure probability δ. Let v_i be the node in G whose SimRank similarity to u (denoted by $s(u, v_i)$) is the i-th largest, $i \in [1, k]$. A top-k SimRank query returns a set of k nodes $V'_k = \{v'_1, \ldots, v'_k\}$, such that with at least $1 - \delta$ probability, for any $k \in [1, n)$, it satisfies that $s(u, v'_i) \geq s(u, v_k) - \varepsilon_{min}$ for all $i \in [1, k]$, where ε_{min} is a very small error tolerance parameter.*

Definition 2 (Thresholding Query). *Given a node u in G, a real number $\tau \in [0, 1]$, and a failure probability δ, denote by V_τ the set of nodes with SimRank similarity no smaller than τ w.r.t. u, i.e., $V_\tau = \{v | s(u, v) \geq \tau, v \in V\}$. A thresholding SimRank query returns a set of nodes V'_τ, such that with $1 - \delta$ probability, for any v with $s(u, v) \geq \tau + \varepsilon_{min}$, v is included in V'_τ; and for any v with $s(u, v) \leq \tau - \varepsilon_{min}$, v is excluded from V'_τ. Here, ε_{min} is a very small error tolerance parameter.*

In this paper, we set $\varepsilon_{min} = 10^{-6}$ for the following reasons. First, even the *exact* algorithm (e.g., the *Power Method*) needs ε_{min} to guarantee its convergence, and computes an approximation $\hat{s}(u, v)$ such that $|\hat{s}(u, v) - s(u, v)| \leq \varepsilon_{min}$. Second, our setting of

[1]Throughout this paper, we use the term single-pair and single-source query to denote the computation of SimRank with up to an additive error, due to the recursive nature of SimRank definition. They are also referred to as the *approximate* single-pair and single-source queries in [24, 30, 32].

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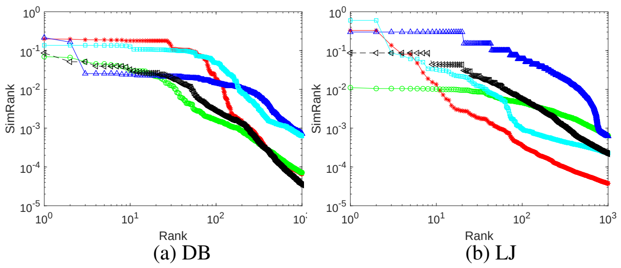
Table 1: A toy example with query node u_1 and u_2, where $s(*, *)$ (resp. $\hat{s}(*, *)$) denotes the exact (resp. estimated) SimRank values ($\varepsilon = 0.05$)

Node	$s(u_1, v)$	$\hat{s}(u_1, v)$
v_1	0.28	0.3
v_2	0.26	0.25
v_3	0.08	0.1
v_4	0.06	0.05

Node	$s(u_2, v)$	$\hat{s}(u_2, v)$
v_1	0.09	0.085
v_2	0.08	0.1
v_3	0.07	0.09
v_4	0.065	0.06



(a) DB (b) LJ

Figure 1: The distribution of top-1000 largest SimRank values for five random query nodes. For each SimRank value, the estimation error is below 10^{-6}.

ε_{min} is orders of magnitude smaller than the state-of-the-art single-source algorithms [24, 30, 32], which are the baselines that achieve the best query performance for top-k and thresholding SimRank queries. Finally, as shown later, the MAB algorithms [12, 19, 26] also need such an error parameter, to the best of our knowledge.

Motivations. Although single-pair and single-source queries have been extensively studied, very few works directly consider the top-k or thresholding queries. The only known method is *TopSim* [21], which is specially designed for top-k queries. *TopSim* estimates similarity values by forward (i.e., following in-edges) and then backward (i.e., following out-edges) traversals level by level from the query node. A stopping rule is used to speculate if the k-th largest estimated SimRank value is larger than the *heuristic* upper bound of the $k+1$-th to the $|V|$-th largest ones. However, the heuristics sacrifices the query accuracy for speed, and always leads to inferior answer quality. On the other hand, algorithms for single-source queries [17, 24, 28, 30, 32] can naturally be extended to answer top-k and thresholding queries following the *return all and postprocessing* paradigm. For example, to answer top-k queries it first computes an approximate similarity for each node, followed by sorting all estimations and returns the nodes with top-k largest SimRank values. Among them, the algorithms [24, 30, 32] with absolute error guarantee achieve state-of-the-art performance.

Nonetheless, all these algorithms suffer from a few deficiencies in answering the top-k or thresholding queries. First, most of them [17, 28, 30, 32] are index-based, which pre-compute a fraction of the intermediate results to accelerate query-time performance. As a consequence, they have quite limited flexibility to answer SimRank queries on dynamic graphs or with the user-defined error parameter. Second, the absolute error guarantee of the single-source query turns out to have little correlation with the answer quality of top-k and thresholding queries. As an example, Table 1 demonstrates the similarity of four nodes $\{v_1, v_2, v_3, v_4\}$ w.r.t. query node u_1 and u_2. Although the estimation achieves an absolute error of 0.05, the precision of the top-2 query varies significantly (1 vs. $\frac{1}{2}$). To the best of our knowledge, no single-source algorithm can achieve acceptable answer quality with reasonable query speed, even on a million-node graph.

Contributions. In this paper, we improve both the query efficiency and effectiveness of top-k and thresholding SimRank queries in a unified manner. We refer to the algorithm as *SimTab* (SimRank queries with Tighter confidence bounds and multi-armed bandits), which is sampling-based and depends on the random walk interpretation of SimRank. In particular, we model the top-k and thresholding queries from the perspective of the Multi-Armed Bandit (MAB) problems. The MAB problem takes a set of n arms as input, while each sample of an arm yields a reward in $[0, 1]$, which is generated randomly following a fixed distribution associated with the arm. Based on this, a bunch of problems [7] have been proposed and well studied, such as the top-k arm identification problem, which aims to find the arms with top-k largest rewards by as few samples as possible. Since existing SimRank algorithms [10, 17, 28] answer SimRank query by generating random walks from the corresponding nodes repeatedly and independently, the related SimRank queries can be naturally modeled as the corresponding MAB problems. However, these algorithms treat each node equally, i.e., each node is sampled the same times. By integrating the arms sampling strategies, our algorithm treats each node differently by their SimRank values in the sampling procedure, which significantly improves the sample complexity. For our proposed method, the query complexity is dependent on the hardness of the query instance and closely matches the theoretical sampling complexity for the corresponding MAB problem. In particular, given a query node u, the hardness of the top-k query is determined by $H_k = \sum_{v \in V} \frac{1}{\Delta_v{}^2}$, where intuitively Δ_v denotes the gap between $s(u, v)$ and the k-th largest SimRank w.r.t. u. As for the thresholding query with parameter τ, the hardness is described by $H_\tau = \sum_{v \in V} \frac{1}{\Delta_{\tau,v}{}^2}$, whereas $\Delta_{\tau,v} = |s(u, v) - \tau|$ for each node v.

Notably, we observe that the SimRank similarities have skewed distribution in most cases, partially due to the power-law distribution of real-world graphs[2]. Meanwhile, the absolute SimRank values for different query nodes also vary dramatically (shown in Figure 1). This phenomenon produces a great influence on the problem complexity as the query parameter varies. For example, nodes with small SimRank values are hard to be distinguished from each other since the gap between them is small. Hence, a large number of samples are needed for top-k queries with large k, or thresholding queries with small τ. To improve the practical efficiency, we propose a novel sampling strategy specially tailored for SimRank queries, for that the MAB algorithms have severe scalability problems on large-sized graphs. We employ several techniques to tighten the confidence bound in SimRank estimation, including the empirical Bernstein inequality [27], a few variance reduction tricks, and careful algorithm design. It turns out that the tightness of confidence bound not only improves the accuracy of SimRank estimation, but also has a major effect on the practical efficiency of the algorithms. Our algorithms are the first to answer *exact* top-k and thresholding queries, i.e., the query result can be at least as good as the *Power Method* [16], which is taken as the ground truth [24, 30]. Last but not least, our algorithms are index-free, which can be naturally applied to dynamic graphs. Table 2 compares our proposed algorithms with state of the art.

Finally, we conduct extensive experiments to evaluate our algorithms against state-of-the-art methods on several large datasets. For both top-k and thresholding queries, we provide the first detailed analysis to demonstrate the performance of existing algorithms on different query parameters (i.e. k and threshold τ). Specifically, we adopt Precision@k to evaluate the quality of top-k query results, while for thresholding queries, we measure precision, recall, and F1-score. We also empirically demonstrate that

[2]We use this term to describe the skewed distribution observed in a variety of networks.

Table 2: Comparison of SimRank algorithms for top-k and thresholding queries. For the empirical performance, non-stable means the evaluation metric (e.g., Precision@k for top-k queries) fluctuates when varying the query parameters (k and τ). Note that the complexity of the MAB algorithms for top-k and thresholding queries are $O(H_{k,\varepsilon_{min}} \log \frac{n}{\delta})$ and $O(H_{\tau,\varepsilon_{min}} \log \frac{n}{\delta})$, respectively. (See Section 2.4 for definition of $H_{k,\varepsilon_{min}}$ and $H_{\tau,\varepsilon_{min}}$.) Therefore, our proposed algorithms also improve the theoretical efficiency.

Method	Query Complexity	Index Cost (Space, Time)	Theoretical Guarantee	Empirical Performance
TopSim [21]	$O(\bar{d}^{2l})$	N/A	N/A	Non-stable
TSF [28]	$O(R_g R_q T^2)$	$O(R_g \lvert V \rvert)$	N/A	Non-stable
SLING [30]	$O(\frac{n}{\varepsilon})$ or $O(m\log^2 \frac{1}{\varepsilon})$	$O(\frac{n}{\varepsilon}), O(\frac{m}{\varepsilon} + \frac{n}{\varepsilon^2} \log \frac{n}{\delta})$	Absolute error	Non-stable
ProbeSim [24]	$O(\frac{n}{\varepsilon^2} \log \frac{n}{\delta})$	N/A	Absolute error	Non-stable
READS [17]	$O(\frac{n}{\varepsilon^2} \log \frac{n}{\delta})$	$O(\frac{n}{\varepsilon^2} \log \frac{n}{\delta})$	Absolute error	Non-stable
PRSim [32]	$O(\frac{n}{\varepsilon^2} \log \frac{n}{\delta} \cdot \sum_{w \in V} \pi(w)^2)$	$O(\min(\frac{n}{\varepsilon}, m)), O(\frac{m}{\varepsilon})$	Absolute error	Non-stable
SimTab-Top-k	$\min(O(\frac{\theta}{{\varepsilon_{min}}^2} \log \frac{n}{\delta}), O(H_{k,\varepsilon_{min}} \log \frac{n}{\delta}))$	N/A	Exact answer	Good and stable
SimTab-Thres	$\min(O(\frac{\theta}{{\varepsilon_{min}}^2} \log \frac{n}{\delta}), O(H_{\tau,\varepsilon_{min}} \log \frac{n}{\delta}))$	N/A	Exact answer	Good and stable

the query accuracy does not have a direct correlation with the absolute estimation error. For all studied experiments, our algorithms significantly outperform existing methods in terms of both practical efficiency and effectiveness. In particular, all existing methods fail to answer both queries with acceptable query time and result quality even on a million-node graph, while our algorithms are able to return the exact query result with reasonable speed on billion-edge graphs.

2. PRELIMINARIES

Table 3 shows the notations that are frequently used in the remainder of the paper.

Table 3: Table of notations.

Notation	Description
$G(V, E)$	Graph G with vertex set V and edge set E
n, m	Numbers of nodes and edges in G
$I(v), O(v)$	In-neighbor/out-neighbour set of a node v in G
$s(u, v)$	SimRank similarity between two nodes u and v in G
$\hat{s}(u, v)$	Estimation of $s(u, v)$
$W(u)$	A $\sqrt{c}$-walk from a node u
c	Decay factor in the definition of SimRank
ε, δ	Additive error parameter and failure probability
$\beta(v)$	Confidence interval of the estimated similarity of node v, i.e., with high probability $\hat{s}(u, v) - \beta(v) \le s(u, v) \le \hat{s}(u, v) + \beta(v)$
t_a, t_o	The running time of one sample-all-arms (resp. sample-one-arm) operation
θ	t_a / t_o

2.1 SimRank with Random Walks

As indicated in [16], SimRank similarities can be interpreted with coupled random walks. In particular, let u and v be two nodes in G, and $I(u)$ (resp. $I(v)$) be a random walk from u that follows a randomly selected incoming edge at each step. Let t be the step that $I(u)$ and $I(v)$ *first meet*, we have

$$s(u, v) = \mathbb{E}[c^{t-1}], \tag{2}$$

where c is the decay factor in the definition of SimRank (see Equation 1). Subsequent work [17, 30] demonstrate that Equation 2 can be simplified by considering the probabilistic stop at each step. For example, the $\sqrt{c}$-*walk* [30] is defined as follows.

DEFINITION 3 ($\sqrt{c}$-WALK). *Given a node u in G, a $\sqrt{c}$-walk from u is a random walk that follows the incoming edges of each node and stops at each step with $1 - \sqrt{c}$ probability.* □

Consequently, two $\sqrt{c}$-walks $W(u) = (w_0 = u, \ldots, w_l, \ldots)$ and $W(v) = (w'_0 = v, \ldots, w'_l, \ldots)$ from u and v meet if there exists some l such that $w_l = w'_l$. According to [30],

$$s(u, v) = \Pr[W(u) \text{ and } W(v) \text{ meet}]. \tag{3}$$

Based on this random walk interpretation of SimRank, the Monte Carlo approach [10, 17, 30] estimates $s(u, v)$ as follows. The algorithm generates n_r coupled $\sqrt{c}$-walks from u and v, respectively. Let $n_{r,meet}$ be the number of $\sqrt{c}$-walk pairs that meet, then $\frac{n_{r,meet}}{n_r}$ is used as an estimation of $s(u, v)$. The estimation error is guaranteed by the Chernoff-Hoeffding inequality [17, 30].

LEMMA 1 (CHERNOFF-HOEFFDING INEQUALITY [14]). *Let $X_1, \ldots, X_{n_r}$ be independent random variables where X_i is strictly bounded by the interval $[a_i, b_i]$ for every $i \in [1, n_r]$. Let $\bar{X} = \frac{1}{n_r} \sum_{i=1}^{n_r} X_i$. Then*

$$\Pr[|\bar{X} - \mathrm{E}[\bar{X}]| \ge \varepsilon] \le 2\exp\left(-\frac{2{n_r}^2 \varepsilon^2}{\sum_{i=1}^{n_r} (b_i - a_i)^2}\right). \tag{4}$$

Since each pair of walks gives an unbiased estimation of the SimRank value, we have $\mathrm{E}[\bar{X}] = s(u, v)$. Given n_r and the constraint on failure probability, i.e., $\Pr[|\bar{X} - s(u, v)| \ge \varepsilon] \le \delta$, we have $\beta_{n_r} = |\bar{X} - s(u, v)| \ge \sqrt{\frac{1}{2n_r} \log \frac{2}{\delta}}$. We refer to β_{n_r} as the *confidence interval*, which means that with $1-\delta$ probability $s(u, v)$ falls into $[\bar{X} - \beta_{n_r}, \bar{X} + \beta_{n_r}]$. In particular, $\bar{X} - \beta_{n_r}$ (resp. $\bar{X} + \beta_{n_r}$) is referred to as the lower (resp. upper) confidence bound. It can be shown that when $n_r \ge \frac{1}{2\varepsilon^2} \log \frac{2}{\delta}$, with at least $1 - \delta$ probability we have $\left|\frac{n_{r,meet}}{n_r} - s(u, v)\right| \le \varepsilon$. In addition, the expected time required to generate n_r $\sqrt{c}$-walks is $O(n_r)$, since each $\sqrt{c}$-walk has $\frac{1}{1-\sqrt{c}}$ nodes in expectation. Therefore, the expected time complexity of answering a single-pair query is $O(\frac{1}{\varepsilon^2} \log \frac{1}{\delta})$.

Note that *MC* can be straightforwardly extended to answer single-source queries by conducting single-pair query for each node $v \in V \backslash \{u\}$ and the query node u. To guarantee the absolute estimation error ε for every node v with at least $1 - \delta$ probability, by the union bound the complexity is $O(\frac{n}{\varepsilon^2} \log \frac{n}{\delta})$, where n denotes the number of vertices in G. Since each node has to generate a large number of $\sqrt{c}$-walks, this approach incurs considerable query overheads for large graphs, and is practically infeasible.

2.2 The Forward and Backward Random Walk Scheme

To improve the practical efficiency of the Monte Carlo method for single-source queries, a few works [17, 21, 24, 28, 30, 32] have been recently proposed based on the random walk interpretation of SimRank. We unify them as *the forward and backward random walk scheme*, as listed in Table 4. Generally speaking, all these methods contain two stages in the SimRank computation, i.e., the *forward* stage and the *backward* stage, while both stages can be implemented in a deterministic or randomized way. Specifically, the deterministic computation relies on the following equation, which enumerates all coupled *similarity paths* [21] from u and v that meet:

$$s(u,v) = \sum_{t=1}^{\infty} \sum_{w \in V} p_{ft}(u,v,w) \cdot c^t. \tag{5}$$

Here, we denote by $p_{ft}(u,v,w)$ the probability of two random walks from u and v first meet at w. On the other hand, the randomized computation is based on Equation 3. In the forward stage, the algorithm deterministically enumerates all reachable nodes w from the query node u following *in-edges*, or randomly samples a subset from them. In the backward stage, from each w a deterministic or randomized traversal following *out-edges* is conducted to reach a set of nodes v, and we can estimate $s(u,v)$ accordingly. By implementing the forward and backward stage with different strategies, the efficiency and effectiveness of SimRank computation vary significantly. We will discuss the key idea of existing solutions in Section 5.

2.3 The Relation between SimRank and Personalized PageRank

Inspired by [30], *PRSim* [32] proposes a new interpretation of SimRank, where $s(u,v)$ is closely related to the reverse Personalized PageRank of both u and v. Formally, we have the following Equation:

$$s(u,v) = \frac{1}{(1-\sqrt{c})^2} \sum_{l=0}^{\infty} \sum_{w \in V} \pi_l(u,w)\pi_l(v,w)d(w). \tag{6}$$

Here, $\pi_l(u,v)$ is the l-hop Reverse Personalized PageRank (RPPR) from u to v, i.e., the probability of an $\sqrt{c}$-walk from u stopping at v with exact l steps ("reverse" means that each step of the walk follows in-edges), while $d(w)$ represents the probability that two $\sqrt{c}$-walks starting from w never meet again [30]. As we will see in Section 3 and 4, this interpretation enables us to apply a few techniques to significantly tighten the confidence bound in SimRank estimation, such as the forward push [5].

Forward push [5]. The forward push is proposed to compute the Personalized PageRank deterministically. Specifically, let $\pi(s,t)$ denote the PPR values between the source node s and the target node t, which represents the probability of an $\sqrt{c}$-walk from s stopping at t. To estimate $\pi(s,t)$, we initialize the *reserve* $\hat{\pi}_f(s,v) = 0$ for each $v \in V$, which is an underestimation of $\pi(s,v)$. Meanwhile, we initialize the residue $r_f(s,v) = 0$ for $v \in V \backslash \{s\}$ and $r_f(s,s) = 1$. Intuitively, $r_f(s,v)$ denotes the probability staying at node v that has not been handled yet. The push operation on a node v first transmits $1-\sqrt{c}$ fraction of its residue to its reserve, then evenly distributes the remaining residue to its our neighbors. This process can be formulated by the following Equation: $\hat{\pi}_f(s,v) \leftarrow \hat{\pi}_f(s,v) + (1-\sqrt{c})r_f(s,v), r_f(s,u) \leftarrow r_f(s,u) + \frac{\sqrt{c}}{|O(v)|} r_f(s,v), \forall u \in O(v)$. As more push operations are conducted, the residues are transferred into the reserves, resulting in a more accurate estimation of $\pi(s,t)$. The following Equation holds in any step of forward push, for $s,t \in V$: $\pi(s,t) = \hat{\pi}_f(s,t) + \sum_{v \in V} r_f(s,v)\pi(v,t)$. We omit the subscripts when the context is clear.

2.4 The Multi-Armed Bandits Problem

In this paper, we answer top-k and thresholding SimRank queries by modeling them as the corresponding multi-armed bandits (MAB) problems. We briefly describe the problem setting as follows. The MAB problem considers an arbitrary instance of an n-armed bandit ($n \geq 2$). Each arm a is associated with a fixed but unknown distribution with expected reward $p_a \in [0,1]$, while each sample (or "pull") of the arm yields a reward generated randomly from it. The rewards for different trials of an arm or between different arms are mutually independent.

A variety of MAB problems have been extensively studied in the field of theoretical computer science, such as regret minimization [6] and pure exploration [7]. For the latter, it considers finding the best set of arms meeting some specific criteria via the minimum number of arm pulls. In particular, the top-k arm identification [12, 15, 19] problem finds the top-k arms with the largest rewards.

DEFINITION 4 (THE TOP-k ARM IDENTIFICATION PROBLEM [7]). *Given n arms and a failure probability δ, find k arms that have the top-k largest rewards, by using as few samples (i.e. pull of arms) as possible, with at least $1-\delta$ success probability.*

We will demonstrate (later in Section 3.1) how to convert SimRank computation to the MAB problems through its random walk interpretation. In this paper, we also show that the thresholding SimRank queries can be modeled as the following MAB problem, which returns all arms with expected reward above some threshold.

DEFINITION 5 (THE THRESHOLDING BANDITS PROBLEM [7, 26]). *We are given a set of n arms and a failure probability δ. Find all arms that have estimated rewards above a given threshold τ, by using as few samples as possible.*

Sampling complexity. It has been shown [7, 19, 26] that the minimum number of arm pulls (i.e., the sampling complexity) for MAB is determined by the expected reward of each arm. Specifically, for the top-k problem, the sampling complexity is defined as $H_k = \sum_{i=1}^{n} \frac{1}{\Delta_i^2}$ [19], where

$$\Delta_i = \begin{cases} p_i - p_{k+1}, & \text{if } i \leq k; \\ p_k - p_i, & \text{if } i > k. \end{cases} \tag{7}$$

Intuitively, Δ_i characterizes the hardness to differentiate the i-th arm a_i from the actual top-k results. Here, for simplicity of notation, we assume an indexing of the arms such that $p_1 \geq p_2 \geq \ldots \geq p_n$. Similarly, the sample complexity of the thresholding bandits problem can be defined as $H_\tau = \sum_{i=1}^{n} \frac{1}{\Delta_{\tau,i}^2}$ [7, 26], where $\Delta_{\tau,i} = |p_i - \tau|$ is the gap between the reward of the i-th arm and the given threshold.

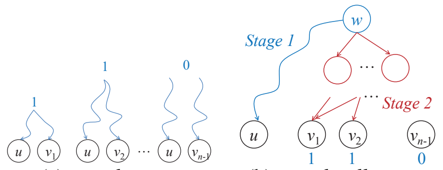
We also note that *all* existing MAB solutions [12, 19, 26] introduce a small error parameter ε_{min} to guarantee that the sampling-based procedure can terminate in extreme cases, e.g., several arms have (nearly) identical expected reward. In this way, arms with expected rewards no smaller than ε_{min} from the actual answer are also considered correct. Correspondingly, the sampling complexity for top-k (resp. thresholding) queries is defined as $O(H_{k,\varepsilon_{min}}) = O((\sum_{i=1}^{n} \frac{1}{\max(\Delta_i, \varepsilon_{min})^2}))$ [12, 19] (resp. $O(H_{\tau,\varepsilon_{min}}) = O((\sum_{i=1}^{n} \frac{1}{(\Delta_{\tau,i}+\varepsilon_{min})^2}))$ [26]).

3. TOP-K QUERIES

3.1 Sampling Strategy in SimRank Computation: from the Perspective of MAB

Table 4: Algorithms following the forward and backward random walk scheme.

Method	The forward stage	The backward stage
TopSim [21]	similarity path enumeration	similarity path enumeration
TSF [28]	random walk sampling	similarity path enumeration (on the indexed one-way graph)
SLING [30]	similarity path enumeration (with pruning)	similarity path enumeration (with pruning)
ProbeSim [24]	$\sqrt{c}$-walk sampling	deterministic or randomized path enumeration, i.e., *DeterministicProbe* or *RandomizedProbe*
READS [17]	(SimRank-aware) random walk sampling	(SimRank-aware) random walk sampling and indexing
PRSim [32]	$\sqrt{c}$-walk sampling	deterministic or randomized path enumeration, e.g., *Variance Bounded Backward Walk*



(a) *sample-one-arm* (b) *sample-all-arms*

Figure 2: The sampling strategies for SimRank: *sample-one-arm* vs. *sample-all-arms*.

3.1.1 *Modeling SimRank computation via MAB*

In this section, we demonstrate how to model the top-k SimRank query as the corresponding top-k arm identification problem from the perspective of multi-armed bandits. Given a query node u, for all nodes $V\backslash\{u\} = \{v_1, \ldots, v_{n-1}\}$, we construct $n-1$ arms with expected reward $s(u, v_1), \ldots, s(u, v_{n-1})$. Note that the expected reward of each arm is not known to the algorithm, but can be estimated via sampling according to the random walk interpretation of SimRank. To be precise, for each v_i, a "pull" of the arm is implemented by sampling a pair of $\sqrt{c}$-walks from the query node u and v_i, respectively (Figure 2(a)). The result of each sampling is either 0 or 1, and gives an unbiased estimation of $s(u, v_i)$ [24,30]. Therefore, designing an efficient top-k SimRank algorithm is equivalent to finding top-k arms with the largest rewards by using as few samples as possible, i.e., the *top-k arm identification* problem [12, 19]. We refer to this sampling strategy as *sample-one-arm*, since each arm (i.e., node pair) is sampled independently.

3.1.2 *Sample-all-arms: another arm sampling strategy for SimRank*

Unfortunately, for any known top-k MAB algorithm, each arm needs to be sampled at least once so that the confidence bound can be computed. The cost, however, is unacceptable for the top-k SimRank queries, which contains a large amount of arms (i.e., nodes). In fact, as our empirical analysis shows, even the state-of-the-art MAB algorithms cannot finish in a reasonable time on a graph with million-sized nodes. On the other hand, we notice that there exists another sampling strategy specially tailored for SimRank queries. Recall the forward and backward random walk scheme proposed in Section 2.2. For the algorithms following this paradigm, a few of them [24,32] adopt random walk sampling in the forward stage. To be precise, they first sample a set of random walks, while for each walk, the backward stage computes an estimation of SimRank similarities for *all* nodes. If the estimation is *unbiased* and *bounded*, we can model this forward and backward procedure as the *sample-all-arms* strategy (Figure 2(b)). For real-world graphs following power-law distribution, the distribution of SimRank scores is highly skewed in practice. Hence, the sample-all-arms strategy achieves much superior practical efficiency than applying sample-one-arm strategy for all nodes (e.g., the *MC* algorithm [9]), because only a fraction of nodes can be reached during the backward searching stage. We will demonstrate in Section 3.3 how to design such a procedure to meet this criterion.

```
Algorithm 1: SimTab-Top-k
    Input: Directed graph $G = (V, E)$; $u \in V$; $k \in [1, n)$; failure
           probability $\delta$
    Output: $V_k$, the estimated top-$k$ nodes with largest SimRank
            values
1 $C$ = Prefiltering($G, u, k, \frac{\delta}{2}$);
2 $V_k$ = Top-$k$-Identification($G, u, k, C, \frac{\delta}{2}$);
3 return $V_k$;
```

3.2 Algorithm Overview

We propose *SimTab-Top-k*, a two-phase algorithm that takes the advantages of both sample-one-arm and sample-all-arms strategies. Specifically, our algorithm contains a *prefiltering* phase and a *top-k identification* phase. In the prefiltering phase, we iteratively apply the sample-all-arms strategy to compute the upper and lower confidence bounds for each estimated SimRank value $\hat{s}(u, v)$. Meanwhile, nodes with low SimRank values that make them impossible to be top-k answers are safely pruned. We refer to the set of remaining nodes as the *candidates*. Once the size of the candidate set is small enough so that applying the sample-one-arm strategy for each candidate is more economical, we stop the prefiltering phase and proceed to the top-k identification phase. Then, a MAB-based algorithm is invoked to keep sampling the nodes independently and following a specified strategy, until we are confident to separate the top-k nodes from other candidates. In this way, the algorithm has at least an identical complexity to the top-k bandits algorithm but achieves much more efficiency in practice.

The pseudo-code is illustrated in Algorithm 1. We first invoke the *Prefiltering* algorithm, which guarantees to return a candidate set C which contains *all* actual top-k nodes with at most $\frac{\delta}{2}$ failure probability. Next, we invoke the *Top-k-Identification* algorithm which finds top-k nodes among the candidates, again with at most $\frac{\delta}{2}$ failure probability. Hence, with high probability, *SimTab-Top-k* returns the true top-k results.

3.3 The Prefiltering Phase

In this section, we propose a *prefiltering* algorithm that can efficiently prune nodes with low SimRank similarities, which is illustrated in Algorithm 2. We adopt an iterative process to continuously apply the sample-all-arm strategy (Lines 3-5), of which the implementation will be amplified later. Specifically, we invoke the sample-all-arms operation 2^{i-1} times in the i-th iteration. For each iteration, the estimated SimRank value $\hat{s}(u, v)$ and confidence interval $\beta(v)$ of every node v are computed from all previously conducted sample-all-arms operations. After that, the top-k nodes with the largest empirical means are added to the candidate set (Line 6). Then, we find the node v' with the smallest lower confidence bound, i.e., $\hat{s}(u, v) - \beta(v)$ (Line 7). Next, we check for each $v \in V\backslash(\{u\} \cup C)$ if it can be pruned from the top-k answers

Algorithm 2: Prefiltering

```
Input: $G = (V, E)$; $u \in V$; $k$; failure probability $\delta$;
Output: Candidate node set $C$
1  Initialize $n_r = 0, numSample = 1$;
2  while true do
3      for $i = 1$ to $numSample$ do
4          $R$ = Sample-all-arms($G, u$);
5          Update $\hat{s}(u, v)$ and $\beta(v)$ for every $v \in V$ with $R$;
6      Let $C = \{v_1, \ldots, v_k\}$ be the nodes with top-$k$ empirical means;
7      Let $v' = \text{argmin}_v\{\hat{s}(u, v) - \beta(v)\}, v \in C$;
8      for each $v \in V \backslash (\{u\} \cup C)$ do
9          if $\hat{s}(u, v') - \beta(v') + \varepsilon_{min} \leq \hat{s}(u, v) + \beta(v)$ then
10             $C = C \cup \{v\}$;
11     if $|C| t_o \leq t_a$ then
12         return $C$;
13     else if $\max_{v \in C} \beta(v) \leq \varepsilon_{min}$ then
14         Sort $C$ according to the empirical means;
15         return the first $k$ nodes in $C$, and skip the top-$k$ identification phase;
16     Increase $n_r$ by $numSample$ and double $numSample$;
```

Algorithm 3: Sample-all-arms

```
Input: $G = (V, E)$; query node $u$;
Output: $R = \{(v, Score(u, v))\}$, a set of nodes with
        non-zero estimated SimRank values
1  Sample an $\sqrt{c}$-walk $W(u) = (w_0 = u, \ldots, w_l)$ from $u$;
2  Sample two independent $\sqrt{c}$-walks $W_1(w_l)$ and $W_2(w_l)$ from $w_l$;
3  if $W_1(w_l)$ and $W_2(w_l)$ do not meet then
4      Initialize hash set $H_j$ for $j = 0, \ldots, l - 1$;
5      Insert $(w_l, 1)$ to $H_0$;
6      for $j = 0$ to $l - 2$ do
7          if $\sum_{x \in H_j} |O(x)| < n$ then
8              $U = \cup_{x \in H_j} O(x)$;
9          else
10             $U = V \backslash \{u\}$;
11         for each $y \in U$ do
12             Uniformly sample an edge $(x, y)$ from $I(y)$;
13             if $x \in H_j$ then
14                 Insert $y$ to $H_{j+1}$ with probability $\sqrt{c}$;
15     return $R = \{(v, \frac{1}{(1-\sqrt{c})^2}) | v \in H_{l-1}\}$;
```

(Lines 8-10). Specifically, we have the following pruning rule, of which the correctness can be easily derived.

The pruning rule. If $\hat{s}(u, v') - \beta(v') + \varepsilon_{min} > \hat{s}(u, v) + \beta(v)$ for some node v, it means that with at least $1 - \delta'$ probability $\min_{v' \in C} s(u, v') + \varepsilon_{min} > s(u, v)$ holds, i.e., v can not be in top-k answer, and will be safely pruned.

For the computation of confidence interval, we use the empirical Bernstein inequality [8]. Intuitively, it states that if the empirical variance is small, then the confidence interval is reversely related to the number of samples n_r. This bound is significantly tighter than that of the Chernoff-Hoeffding inequality, which is in reverse proportional to $\sqrt{n_r}$.

LEMMA 2 (EMPIRICAL BERNSTEIN INEQUALITY [8]). *For any set $\{X_i\}$ ($i \in [1, t]$) of i.i.d. random variables with mean μ and $X_i \in [0, R]$, with $1 - \delta$ probability,*

$$\left|\bar{X}_t - \mu\right| \leq \hat{\sigma}_t \sqrt{\frac{2 \ln 3/\delta}{t}} + \frac{3R \ln 3/\delta}{t}, \tag{8}$$

where $\bar{X}_t = \sum_{i=1}^{t} X_i/t$ is the empirical mean of $\{X_i\}$, and $\hat{\sigma}_t = \sqrt{\frac{1}{t}\sum_{i=1}^{t}(X_i - \bar{X}_t)^2}$ is the empirical standard deviation of $\{X_i\}$.

Hence, the confidence bound is set to $\beta(v) = \hat{\sigma}(v)\sqrt{\frac{2 \ln 3n/\delta}{n_r}} + \frac{3 \ln 3n/\delta}{n_r}$, where n_r is the total number of sample-all-arms operation ever conducted.

The stopping condition. Now we return back to the prefiltering algorithm and explain its stopping condition. We set the stopping condition as $|C| t_o \leq t_a$ (Line 11), where t_a (resp. t_o) denote the expected running time of one sample-all-arms (resp. sample-one-arm) operation. (Note that the cost of a single sample-one-arm operation is asymptotically identical to one $\sqrt{c}$-walk generation.) Therefore, $|C| t_o$ denotes the cost of applying sample-one-arm strategy to each candidate node, and the prefiltering algorithm stops when applying sample-one-arm strategy on *all* candidates is more efficient.

When the stopping condition is not satisfied but the confidence interval of *every* candidate is below ε_{min} (Line 13), the algorithm can still safely terminates. To this end, the prefiltering algorithm computes an approximate SimRank with absolute error ε_{min} for every candidate node. We sort all node in C by descending order of the estimated SimRank values, and return the top-k largest nodes as the final answer (i.e., the top-k-identification phase is skipped). Lastly, if the algorithm cannot finish in this round, we double the number of sample-all-arm operations, and proceed to the next iteration (Line 16).

The *Sample-all-arms* algorithm. The implementation of the sample-all-arms operation is demonstrated in Algorithm 3. It generates a $\sqrt{c}$-walk $W(u) = (w_0 = u, ..., w_l)$, and then samples two $\sqrt{c}$-walks $W_1(w_l)$ and $W_2(w_l)$ from w_l. If the walks do not meet, we invoke a backward traversal procedure from w_l (Lines 4-14). Intuitively, the traversal guarantees that for each $v \in V \backslash \{u\}$, the probability of v contained in H_{l-1} equals the probability that a $\sqrt{c}$-walk from v stops at w_l. Note that by sampling two walks from w_l, we can get an unbiased estimation of $d(w_l)$. Hence, by Equation 6, the Sample-all-arms algorithm computes an unbiased estimation of $s(u, v)$ for *each* v.

Remarks. Indeed, the procedure shares some similar ideas with *RandomizedProbe* in [24] and *Variance Bounded Backward Walk* in [32], but has one key difference. Note that both *Randomized-Probe* and *Variance Bounded Backward Walk* give *unbounded* estimators of the SimRank value. In contrast, our backward traversal procedure returns a 0/1 estimator. Therefore, concentration bounds such as the empirical Bernstein inequality can be easily applied.

Algorithm correctness. We formally prove the correctness of the prefiltering algorithm, which guarantees that all actual top-k nodes are contained in the returned candidate set with high probability. For space constraints, all proofs in our paper are referred to its full version [1]. The following lemma guarantees the effectiveness of the *Sample-all-arms* algorithm.

LEMMA 3. *For each node $v \in V \backslash \{u\}$,* Sample-all-arms *returns an unbiased estimator of $s(u, v)$ that falls in* $[0, 1]$.

From the above lemma and the pruning rule of the prefiltering algorithm, we have the following theorem.

THEOREM 1. *With at least $1 - \delta$ probability, the prefiltering algorithm guarantees that the returned candidate set C contains all actual top-k nodes.*

3.4 The Top-k Identification Phase

3.4.1 Baseline algorithm

In the top-k identification phase, we try to select the top-k nodes by separating them from the candidate nodes that are not likely to be in the top-k answer. We demonstrate how to adapt the MAB algorithms for top-k arm identification to our scenario. We use the UGapEc-V algorithm [12] as an example. The pseudo-code is demonstrated in Algorithm 4. Given graph G, the query node u, an integer k, the candidate set C which contains the estimated SimRank $\hat{s}(u, v)$ and the confidence interval $\beta(v)$ for each candidate v, and a failure probability δ, *Top-k-Identification* returns the actual top-k nodes contained in C. Note that to efficiently update the confidence bound we do not explicitly store $\beta(v)$. For the Chernoff bound, it is sufficient to record $n_r(v)$, the number of samples for node v. If the empirical Bernstein inequality is applied, to compute the empirical variance, we also need to store $\sum_{i=1}^{n_r(v)} \hat{s}_i(u, v)^2$, where $\hat{s}_i(u, v)$ denotes the estimation of $s(u, v)$ in the i-th trial. The algorithm first computes the upper and lower confidence bound for each $v \in C$, denoted as $UB(v)$ and $LB(v)$, respectively. Then, for each C we compute $B(v) = \max^k_{w \in C\backslash\{v\}} UB(w) - LB(v)$, where operator $\max^k_{v \in S} f(v)$ returns the k-th largest value $f(v)$ among all $v \in S$. Intuitively, $B(v)$ represents how bad is a candidate compared to the one with the k-th largest similarity in the worst case. Next, we find the k nodes with smallest $B(v)$, denoted as V_k. Let v_k be the node with the k-th smallest $B(v)$. If $B(v_k) \le \varepsilon_{min}$, we are confident that V_k is the top-k nodes (with additive error ε_{min}). Otherwise, let v_h be the node in V_k having the smallest $LB(v)$, and v_l the node in $C\backslash V_k$ having the largest $UB(v)$. They represent the worst possible arm in V_k and the best possible arm in $C\backslash V_k$, respectively. Then, we sample the arm in $\{v_h, v_l\}$ with the larger confidence interval. Note that each arm sampling is implemented by a coupled random walk from the query node u and the candidate v. Following [12], the confidence bound is computed based on the empirical Bernstein inequality:

$$\beta(v, n_r(v)) = \hat{\sigma}(v, n_r(v)) \sqrt{\frac{\log \frac{|C| r^3}{\delta}}{n_r(v)}} + \frac{\frac{7}{6} \log \frac{|C| r^3}{\delta}}{n_r(v) - 1}, \quad (9)$$

where $\hat{\sigma}(v, n_r(v))$ denotes the empirical standard variance over $n_r(v)$ estimations, and r the round of iteration.

Running example for Algorithm 4. We use a toy example in Fig. 3(a) to illustrate the arm sampling strategy and the stopping rule for the top-k algorithm. Suppose that for the query node u, there exists a candidate set C of five candidate nodes $\{v_1, \ldots, v_5\}$ after the prefiltering phase, and we aim to find the top-2 nodes with the largest similarity. For each node v_i, let μ_i denote the estimated SimRank score, i.e., $\mu_i = \hat{s}(u, v_i)$, and β_i the corresponding confidence interval. Specifically, we have $\{(\mu_1 = 0.09, \beta_1 = 0.02), (\mu_2 = 0.08, \beta_2 = 0.03), (\mu_3 = 0.07, \beta_3 = 0.03), (\mu_4 = 0.07, \beta_4 = 0.02), (\mu_5 = 0.06, \beta_5 = 0.02)\}$. For convenience, we assume that the candidates are numbered in descending order of the estimated similarities. Note that even these candidates are sampled identical times via the sample-all-arm strategy, their confidence intervals can be different when the empirical Bernstein inequality is applied.

Algorithm 4: Top-k-Identification

```
Input: $G = (V, E)$; $u \in V$; $k$; candidate set
       $C = \{v, \hat{s}(u, v), \beta(v)\}$; failure probability $\delta$;
Output: $V_k$ as the top-$k$ results
1  while true do
2      for each $v \in C$ do
3          Compute $UB(v) = \hat{s}(u, v) + \beta(v)$,
           $LB(v) = \hat{s}(u, v) - \beta(v)$;
4      for each $v \in C$ do
5          Compute $B(v) = \max^k_{w \in C\backslash\{v\}} UB(w) - LB(v)$;
6      Let $V_k$ be the set of $k$ nodes with smallest $B(v)$, and $v_k$ be
       the node with $k$-th smallest $B(v)$;
7      if $B(v_k) \le \varepsilon_{min}$ then
8          return $V_k$;
9      else
10         Let $v_h \in V_k$ be the node with smallest $LB$;
11         Let $v_l \in C\backslash V_k$ be the node with largest $UB$;
12         Sample node $v \in \{v_h, v_l\}$ with the larger $\beta(v)$;
13         Update $\hat{s}(u, v)$ and $\beta(v)$;
```

The algorithm first computes the upper and lower confidence bound for each candidate v_i, denoted as UB_i and LB_i, respectively. In particular, we have $\{(UB_1 = 0.11, LB_1 = 0.07), (UB_2 = 0.11, LB_2 = 0.05), (UB_3 = 0.1, LB_3 = 0.04), (UB_4 = 0.09, LB_4 = 0.05), (UB_5 = 0.08, LB_5 = 0.04)\}$. Second, we compute B_i for each node v_i. Note that for v_1 and v_2 with top-2 largest estimated score, $\max^2_{w \in C\backslash\{v\}} UB(w) = UB_3 = 0.1$, whereas for v_3, v_4 and v_5, $\max^2_{w \in C\backslash\{v\}} UB(w) = UB_2 = 0.11$. (Since v_1 and v_2 have identical upper bound, the tie is broken randomly.) Therefore, we have $\{B_1 = 0.03, B_2 = 0.05, B_3 = 0.07, B_4 = 0.06, B_5 = 0.07\}$. We set V_2 as the two nodes with the smallest B_i, i.e., $V_2 = \{v_1, v_2\}$. Since the second smallest B_i is B_2, and $B_2 = 0.05 > \varepsilon_{min}$, more sample-one-arm operations are needed. We select $v_h = v_2$, the node with the smallest LB from V_2, and $v_l = v_3$, the node with the largest UB from $C\backslash V_2$. Intuitively, v_h denotes the worst top-k candidate , and v_l denotes the best possible candidate not in V_2. Since they have the same confidence interval, we sample v_2 in the next iteration (again, the tie is broken randomly).

Assume that after several rounds of iteration, we have the configuration shown in Fig. 3(b). Again, we compute UB_i, LB_i and then B_i for each candidate v_i. Now we have $B_1 = -0.007, B_2 = 0.017, B_3 = -0.001, B_4 = 0.019$, and $B_5 = 0.031$. Since the second smallest B_i (i.e. B_3) is below zero, we are sure that $\{v_1, v_3\}$ is the top-2 nodes with largest similarity, and the algorithm terminates.

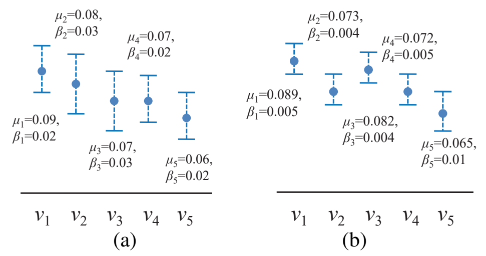


Figure 3: An example for the top-k query.

Analysis. The efficiency of *Top-k-Identification* is bounded by the following lemma.

LEMMA 4. Top-k-Identification *returns the actual top-k nodes with at least* $1-\delta$ *probability and with expected time complexity* $\min\left(O\left(\frac{\theta}{{\varepsilon_{min}}^2}\log\frac{n}{\delta}\right), O\left(\sum_{v\in V\setminus\{u\}}\frac{1}{\max\left(\frac{\Delta_v+\varepsilon_{min}}{2},\varepsilon_{min}\right)^2}\log\frac{n}{\delta}\right)\right)$, *where* $\theta = \frac{t_a}{t_o}$ *denotes the ratio between the time cost of one sample-all-arms operation (i.e.,* t_a*) and one sample-one-arm operation (i.e.,* t_o*).*

We now analyze the expected running time of the *SimTab-Top-k* algorithm.

THEOREM 2. *The* SimTab-Top-k *algorithm answers the top-k SimRank queries with at least* $1-\delta$ *success probability, with asymptotically the same time complexity of* Top-k-Identification.

3.4.2 Optimizations

The *Top-k-Identification* algorithm uses $\sqrt{c}$-walk sampling to estimate the reward of an arm (i.e. the SimRank similarity of a pair of nodes), and always gives 0/1 estimation for each sample-one-arm operation. As a consequence, the empirical variance of the estimation is large, resulting in loose confidence bounds (see Equation 8). Thus, more samples are needed until the stopping condition is satisfied. We propose an optimization algorithm, denoted by *Adaptive-Top-k*. Firstly, we note that SimRank can be interpreted from the perspective of reverse Personalized PageRank, as demonstrated in Equation 6. Instead of using Monte Carlo sampling, the PPR values can also be computed in a deterministic way by forward push [5], which generates estimators with smaller variances but with higher computation cost. Secondly, we conduct the push operation in an adaptive way, i.e., the number of push operations for each candidate varies. Intuitively, for each candidate, we conduct as many forward pushes as possible until the asymptotical complexity of the push operation matches the cost of the walks that has been sampled. Therefore, more push operations are applied to a candidate node if it has been sampled extensively. Note that more push operations significantly tightens the confidence bound. This helps us to effectively distinguish the nodes with SimRank values close to the boundary (i.e., the k-th largest SimRank value or the given threshold), while saving the cost for most other candidates, which guarantees the efficiency of the whole algorithm.

The pseudo-code is demonstrated in Algorithm 5. For each level $l=[0,\infty)$, we first initialize $\hat{\pi}_l(v,w)=0$ for each $v\in C\cup\{u\}$ and $w\in V$. We set $r_0(v,v)=1$ for each $v\in C\cup\{u\}$, and $r_l(v,w)=0$ for each $v\in C\cup\{u\}$ and $w\in V$ for $l\geq 1$. The level information must be recorded to guarantee the walks meet at the same step. Initially, no push operation is performed. For each candidate v, once the number of samples doubled, we conduct a few pushes based on a parameter r_{max}. Intuitively, r_{max} prevents those push operations from nodes with small residues to get a good tradeoff between algorithm efficiency and effectiveness. When we are to estimate the similarity of the query node u and a candidate v, we follow the idea of Equation 6. Combining with the property of forward push, we rewrite the Equation as follows.

$$s(u,v) = a\sum_{l=0}^{\infty}\sum_{w\in V}(\hat{\pi}_l(u,w)+\delta_l(u,w))(\hat{\pi}_l(v,w)+\delta_l(v,w))d(w), \tag{10}$$

where $a=\frac{1}{(1-\sqrt{c})^2}$, $\hat{\pi}_l(s,w)$ is the reserve by forward push, and $\delta_l(s,w)=\sum_{v\in V}\sum_{i=0}^{l} r_i(s,v)\pi_{l-i}(v,w)$. First, we fetch all node w having non-zero estimated reserves from both u and v at each level l, and aggregate them following Equation 10. Next, for both u and v we sample a $\sqrt{c}$-walk to derive an unbiased estimation of $\delta_l(u,w)$ (resp. $\delta_l(v,w)$). Take v as the example, first a node y with $r_{l_2}(v,y)$ is sampled with probability $\frac{r_{l_2}(v,y)}{r_{sum}(v)}$, where $r_{sum}(v)=\sum_l\sum_{w\in V} r_l(v,w)$ denotes the sum of all probabil-

Algorithm 5: Adaptive-Top-k Algorithm

```
Input: $G=(V,E)$; $u\in V$; $k$; candidate set
       $C=\{v,\hat{s}(u,v),\beta(v)\}$; failure probability $\delta$;
Output: $V_k$, the estimated top-$k$ nodes with largest SimRank
        values
1  $n_r(u)=\sum_{v\in C} n_r(v), n'_r(v)=n_r(v), \forall v\in C\cup\{u\}$;
2  for each $v\in C\cup\{u\}$ and $l=0,1,\ldots$ do
3      if $l=0$ then
4          $r_l(v,v)=1, r_l(v,w)=0, \forall w\neq v$;
5      else
6          $\hat{\pi}_l(v,w)=0, r_l(v,w)=0, \forall w\in V$;
7  Let $H_l(v)=\{w|\hat{\pi}_l(v,w)>0\}, R_l(v)=\{w|r_l(v,w)>0\}$;
8  Replace Line 12 of Algorithm 4 into:
9  $\hat{s}(u,v)=0$;
10 for $l=0,1,\ldots$ do
11     for each $w\in H_l(u)\cap H_l(v)$ do
12         Increase $\hat{s}(u,v)$ by $\hat{\pi}_l(u,w)\hat{\pi}_l(v,w)\hat{d}(w)$;
13 Sample an item $(x,r_{l_1}(u,x))$ from $\{R_0(u),R_1(u),\ldots\}$;
14 Sample an $\sqrt{c}$-walk $W(x)$ from $x$, which stops at node $x'$;
15 Let $l'_1=l_1+|W(x)|$;
16 Sample an item $(y,r_{l_2}(v,y))$ from $\{R_0(v),R_1(v),\ldots\}$;
17 Sample an $\sqrt{c}$-walk $W(y)$ from $y$, which stops at node $y'$;
18 Let $l'_2=l_2+|W(y)|$;
19 Let $r_{sum}(u)=\sum_{R_0(u),R_1(u),\ldots}\sum_{x\in V} r_l(u,x)$;
20 Let $r_{sum}(v)=\sum_{R_0(v),R_1(v),\ldots}\sum_{y\in V} r_l(v,y)$;
21 if $\hat{\pi}_{l'_1}(v,x')\neq 0$ then
22     Increase $\hat{s}(u,v)$ by $r_{sum}(u)\hat{\pi}_{l'_1}(v,x')\hat{d}(x')$;
23 if $\hat{\pi}_{l'_1}(u,y')\neq 0$ then
24     Increase $\hat{s}(u,v)$ by $\hat{\pi}_{l'_1}(u,y')r_{sum}(v)\hat{d}(y')$;
25 if $l'_1=l'_2$ and $x'=y'$ then
26     Increase $\hat{s}(u,v)$ by $r_{sum}(u)r_{sum}(v)\hat{d}(x')$;
27 Use $\hat{s}(u,v)$ as an estimation of $s(u,v)$;
28 Insert after Line 13 of Algorithm 4:
29 Increase $n_r(v_h)$ and $n_r(v_l)$ by 1, respectively;
30 Increase $n_r(u)$ by 2;
31 for any $v\in\{v_h,v_l,u\}$ do
32     if $n_r(v)=2n'_r(v)$ then
33         ForwardPush($G,v,\frac{1}{n_r(v)}$);
34         $n'_r(v)=n_r(v)$;
35 ForwardPush($G,v,r_{max}$)
36 for $l=0,1,\ldots$ do
37     for each item $(w,r_l(v,w))\in R_l(v)$ do
38         if $\frac{r_l(v,w)}{|I(w)|}>r_{max}$ then
39             $\hat{\pi}_l(v,w)=\hat{\pi}_l(v,w)+(1-\sqrt{c})\cdot r_l(v,w)$;
40             Update $\hat{\pi}_l(v,w)$ in $H_l(v)$;
41             for each $x\in I(w)$ do
42                 $r_{l+1}(v,x)=r_{l+1}(v,x)+\frac{\sqrt{c}}{|I(w)|}\cdot r_l(v,w)$;
43                 Update $r_{l+1}(v,x)$ in $R_{l+1}(v)$;
44             $r_l(v,w)=0$;
```

ities not handled yet. Then we sample a $\sqrt{c}$-walk from y, which terminates at node y'. Let $l'_2 = l_2 + |W(y)|$. If $\hat{\pi}_{l'_2}(u, y') \neq 0$, we add $\hat{\pi}_{l'_2}(u, y')r_{sum}(v)\hat{d}(y')$ to the estimation, and vice versa for node u. If the walk of u and v meet (i.e., $x' = y'$), we add $r_{sum}(u)r_{sum}(v)\hat{d}(x')$ to $\hat{s}(u, v)$. It can be proved that the estimator is unbiased for $s(u, v)$. For the estimation of $d(w)$, it can be implemented by sampling two $\sqrt{c}$-walks from w, which gives 0/1 estimation.

LEMMA 5. *The time and space complexity of Adaptive-Top-k is asymptotically identical to those of the Top-k-Identification algorithm.*

4. THRESHOLDING QUERIES

In this section, we demonstrate how to adapt our arm sampling strategies and the techniques for confidence bound to thresholding queries, which returns all nodes with SimRank values larger than a threshold τ for a given query node u. Firstly, by tackling the problem from the perspective of MAB, a greedy arm sampling strategy [26] is adopted for the sample-one-arm operations[3]. Secondly, to enhance practical efficiency, we also employ the *sample-all-arms* strategy, which is implemented by the prefiltering algorithm and with a modification of the pruning rule. Our algorithm, denoted as *SimTab-Thres*, is shown in Algorithm 6. Similar to *SimTab-Top-k*, the algorithm contains a prefiltering phase followed by a refinement phase.

Algorithm 6: *SimTab-Thres*

```
   Input: Directed graph $G = (V, E)$; $u \in V$; threshold $\tau$;
          failure probability $\delta$;
   Output: $V_\tau$, the estimated node set with SimRank value no
           smaller than $\tau$
1  $V_\tau = \emptyset$;
2  $C$ = Prefiltering($G, u, \tau, \frac{\delta}{2}$);
3  Initialize minimum queue $Q = \emptyset$;
4  Let $n_r(v)$ be the number of samples of node $v$;
5  for each $v \in C$ do
6      Add $(v, \sqrt{n_r(v)} \cdot |\hat{s}(u, v) - \tau|)$ to $Q$;
7  while $Q \neq \emptyset$ do
8      $(v, p(v))$ = pop($Q$);
9      Sample a pair of $\sqrt{c}$-walks from $u$ and $v$ to update $\hat{s}(u, v)$
       and $\beta(v)$;
10     if $\hat{s}(u, v) - \beta(v) > \tau$ then
11         Add $v$ to $V_\tau$;
12     else if $\beta(v) \leq \varepsilon_{min}$ and $\hat{s}(u, v) > \tau$ then
13         Add $v$ to $V_\tau$;
14     else if $\beta(v) > \varepsilon_{min}$ and $\hat{s}(u, v) + \beta(v) > \tau$ then
15         Update $p(v)$, and put $(v, p(v))$ back into $Q$;
16 return $V_\tau$;
```

The prefiltering phase. In the prefiltering phase (Line 2), we filter out nodes that can not be in V_τ and get a candidate set C. With probability at least $1 - \frac{\delta}{2}$, C contains all nodes in V_τ. Each item in C is represented by a triple $(v, \hat{s}(u, v), \beta(v))$, where $\beta(v)$ denotes the confidence interval and can be updated later in the refinement phase according to the implementation described in Section 3. The prefiltering algorithm is analogous to Algorithm 2 but with the modified pruning rule as follows.

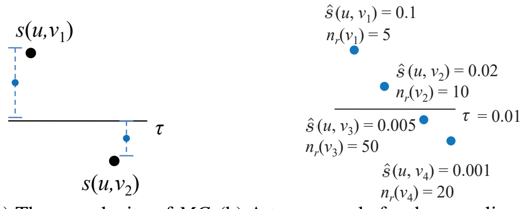
[3]More precisely, in [26] the proposed method solves the thresholding bandit problem under the fixed budget setting, which minimizes the error of estimation given the number of samples. On the other hand, our problem belongs to the fixed confidence setting, i.e., minimizing the number of samples for a predefined failure probability.

The pruning rule. For node v satisfying that $\hat{s}(u, v) - \beta(v) \geq \tau$, we directly add it to V_τ; node v satisfying that $\hat{s}(u, v) + \beta(v) < \tau$ will be discarded. If node v satisfies that $\hat{s}(u, v) - \beta(v) < \tau \leq \hat{s}(u, v) + \beta(v)$, we can not decide whether $v \in V_\tau$. Therefore, it is referred to as the candidate node.

The refinement phase. In the refinement phase, we identify the nodes with SimRank values above τ from C. Intuitively, this can be done by applying the Monte Carlo procedure for each candidate node. For node v, the procedure stops as long as the confidence bound $\beta(v)$ falls below $\frac{|s(u,v)-\tau|}{2}$ (see Figure 4(a)). Moreover, the time complexity asymptotically matches the hardness of the thresholding bandit problem. Nonetheless, we adopt a heuristic adaptive sampling strategy [26], which facilitates the optimization techniques and approximate version of the query. Details are referred to the full version of our paper [1].

The sampling strategy. At every step, we sample the node $v \in C$ with the minimum weight $p(v) = \sqrt{n_r(v)} \cdot |\hat{s}(u, v) - \tau|$.

Once we are sure that $v \in V_\tau$ (Lines 10-11) or the estimation is as accurate as of the ground truth (Lines 12-13), v is moved to V_τ or discarded based on the estimation value. Here, we use a very small error parameter ε_{min} (e.g. 10^{-6}) to handle nodes with $s(u, v) = \tau$. Otherwise, the sampling-based algorithm will not stop for these nodes. The setting of ε_{min} guarantees that our result is at least as good as the ground truth used in [24, 32].



(a) The complexity of *MC*. (b) A toy example for the sampling strategy.

Figure 4: An example for the thresholding query.

Runinng example for Algorithm 6. Consider the toy example in Figure 4(b), where we have four candidates $\{v_1, v_2, v_3, v_4\}$ for the thresholding query with $\tau = 0.01$. Suppose that after several rounds of sample-all-arms and sample-one-arm operations, we have $\{(\hat{s}(u, v_1) = 0.1, n_r(v_1) = 5), (\hat{s}(u, v_2) = 0.02, n_r(v_2) = 10), (\hat{s}(u, v_3) = 0.005, n_r(v_3) = 50), (\hat{s}(u, v_4) = 0.001, n_r(v_4) = 20)\}$. Then, according to the sampling strategy, we compute $p(v_1) = \sqrt{5} \cdot 0.09 \approx 0.201$, $p(v_2) = \sqrt{10} \cdot 0.01 \approx 0.032$, $p(v_3) = \sqrt{50} \cdot 0.005 \approx 0.035$, and $p(v_4) = \sqrt{20} \cdot 0.009 \approx 0.040$. Therefore, v_2 will be chosen since it has the minimum weight. Note that the sampling strategy implies that a candidate v which is sampled few times whereas having a small gap between the estimated value and the threshold should be re-considered. Intuitively, since the gap between v_1, v_4 and τ is sufficiently large, no more sample is needed; meanwhile, a large number of samples has already given an accurate estimation for v_3.

We theoretically prove the correctness and complexity of the *SimTab-Thres* algorithm.

THEOREM 3. *With at least $1 - \delta$ probability,* SimTab-Thres *returns the true V_τ, i.e. the node set with SimRank value* *no smaller than the threshold τ, with expected time complexity* $\min\left(O(\frac{\theta}{\varepsilon_{min}{}^2}\log\frac{n}{\delta}), O(\sum_{v\in V\setminus\{u\}}\frac{1}{(\Delta_{\tau,v}+\varepsilon_{min})^2}\log\frac{n}{\delta})\right)$.

Optimizations. Recall that during the top-k identification phase of *SimTab-Top-k*, we employ an adaptive forward push to tighten the confidence bounds without additional cost. This technique can be integrated into the refinement phase of *SimTab-Thres*, since both queries apply the sample-one-arm strategy in which arms are sampled independently and repeatedly.

5. RELATED WORK

To the best of our knowledge, very few methods are directly developed for the top-k and thresholding SimRank queries. Therefore, we classify the related work into (1) algorithms for top-k queries [21], and (2) the single-source algorithms with the state-of-the-art empirical performance on these queries. We also include a brief discussion of other related work.

5.1 Algorithms for Top-k Queries

TopSim [21] is the only known method that exactly solves the top-k SimRank query. Given the query node u, *TopSim* firstly finds all w reachable from u with exact l steps following *in-edges*, where l starts from 1 and increase by 1 once all such w are found. For each w, it finds all v reachable from w in exact l steps following *out-edges*. Moreover, v must not be any node in path $w \rightsquigarrow u$. Then the probability of $w \rightsquigarrow u, w \rightsquigarrow v$ is aggregated into $\hat{s}(u,v)$, an estimation of $s(u,v)$. The algorithm stops when the gap between k-th and $(k+1)$-th largest score exceeds the heuristic upper bound of the score any node can gain with more than l steps, in fact, $(\frac{c}{\bar{d}})^{l+1}$, where c is the decay factor and $\bar{d}$ is the average degree of the graph. The authors also propose several optimization algorithms to improve the speed, some with trade of accuracy.

5.2 State-of-the-art Single-Source Queries

The recently proposed single-source algorithms [24,32] are state of the art for both top-k and thresholding queries. They all employ the *return all and postprocessing* paradigm, i.e., they first derive an approximate estimation for each node in the graph, followed by returning the set of nodes satisfying the query constraint.

5.2.1 The index-free algorithm

ProbeSim [24] is the state-of-the-art index-free algorithm that is able to compute single-source SimRank queries on large graphs. Given a query node u, *ProbeSim* samples n_r $\sqrt{c}$-walks from u following in-edges in the forward stage. For each walk $W(u) = (w_0 = u, w_1, \ldots)$, let w_l be the node at the l-th step. The algorithm then performs a *probe* procedure from each $w_l(l = 1, \ldots)$ in the backward stage, where the meeting probabilities for different w_i are aggregated to derive an unbiased estimation of $s(u,v)$. They provide both a deterministic and a randomized version of the probe procedure, which is essentially based on deterministic or randomized similar path enumeration.

5.2.2 Index-based algorithms

Most single-source algorithms [17, 28, 30, 32] use index to improve the query performance. In general, they pre-compute a fraction of the results of similarity path enumeration or a large number of random walks during index construction, while the index can be reused in the query phase. *TSF* [28] constructs a set of *one-way graphs* as index via random in-neighbor sampling, and answers single-source queries by online random walk sampling and traversal on one-way graphs. On the contrary, *SLING* [30] implements the forward and backward stage as similarity path enumeration. It computes the *hitting probabilities* from each node v, which denotes the probability of an $\sqrt{c}$-walk from v passing w. Only non-negligible probabilities are indexed to reduce space costs. *READS* [17] proposes an indexing scheme along with the *SimRank-aware random walk* to enhance both theoretical and practical query efficiency of *MC*. As the state-of-the-art index-based approach, *PRSim* [32] improves the efficiency of the backward stage via a probability-guided search of similarity paths. To limit the index space, it only conducts backward search [4] from nodes with high reverse PageRank scores (i.e., PageRank following in-edges). In the query phase, given a $\sqrt{c}$-walk generated in the forward stage, if it stops at a hub node, the indexed estimation values are directly retrieved; otherwise a randomized searching procedure is invoked to estimate the SimRank values, which only incurs sub-linear cost on power-law graphs.

Although pre-computing partial intermediate results as the index benefits the query time performance, it also has several fatal drawbacks. Firstly, all known methods except [17, 28] construct *static* index, which means the index can not be updated once the graph changes. Secondly, for *every* index-based method, the preprocessing phase (e.g., the size of the index) is determined by the error parameter ε, which is user-defined during the query phase. Therefore, these algorithms suffer from low flexibility.

5.3 Other Related Work

The algorithms for SimRank can be broadly divided into the iterative methods and the random walk based methods. [16] proposes the *Power Method*, an iterative method to compute the all-pair SimRank matrix S. It is based on the matrix formulation of SimRank [20]: $S = (cP^{\top}SP) \vee I$, where I is the identity matrix of compatible size, P is a *transition matrix* defined by the edges in G, and $\vee$ is the element-wise maximum operator. A bunch of follow-up work [25, 31, 35, 37] improves its efficiency or accuracy; however, as all methods incur $O(n^2)$ space overheads, the cost is prohibitive for large-sized graphs. We also note a line of research [11, 13, 20, 22, 33, 34, 36] has been proposed with a modified definition of SimRank that makes it easier to compute: $S = cP^{\top}SP + (1-c)\cdot I$. However, [20, 30] prove that this definition is rather different from the original SimRank.

6. EXPERIMENTS

This section experimentally evaluates our proposed algorithms against the state-of-the-art methods for top-k and thresholding SimRank queries.

Table 5: Datasets.

Dataset	Type	n	m
DBLP (DB)	undirected	5,425,963	17,298,033
LiveJournal (LJ)	directed	4,847,571	68,993,773
IT-2004 (IT)	directed	41,291,594	1,150,725,436
Friendster (FD)	directed	68,349,466	2,586,147,869

6.1 Experimental Setup

Datasets. We use four large graph datasets [2,3] with edge numbers varying from tens of millions to billions, as shown in Table 5.

Query generation. We consider two different strategies for query node generation. 1) *Uniformly at random*. Following all previous studies [17, 24, 28, 30, 32], for each dataset, we randomly generate 1,000 query nodes for top-k and thresholding queries, respectively. 2) *Stratified sampling*. Due to the definition of Sim-

Rank, a query node with higher in-degree tends to have more nodes with smaller similarities. We split the in-degrees into intervals $[1, 10), [10, 10^2), [10^2, 10^3), [10^3, 10^4)$ and $[10^4, \infty)$, and generate 100 random queries for each interval. For space constraints, we only report the empirical results under the uniformly-at-random setting, for that the conclusions of two different settings are similar.

Methods. We evaluate our top-k and thresholding algorithm with *ProbeSim* [24], the state-of-the-art index-free algorithm, and the state-of-the-art index-based algorithms, including *PRSim* [32] and *READS* [17]. We include *TopSim* [21] and *TSF* [28] as baselines. Since *PRSim* can be easily modified into an index-free algorithm by setting the number of indexed hubs as 0, we also take it into consideration, and denote it as *PRSim-IF* (for index-free). We also compare our methods to *Opt-LP*, the state-of-the-art all-pair SimRank algorithm [31]. We obtain the code of *ProbeSim*, *READS*, *PRSim*, and *Opt-LP* from the authors, and implement all other algorithms in C++ and compile the codes with -O3 option. All experiments are conducted on a machine with a 2.6GHz CPU and 128GB memory. Following previous works [24, 30, 32], we set $c = 0.6$ through all experiments.

Parameters. For each method, we choose two parameter settings: the *typical* parameter setting following the original paper, and a *precise* parameter setting to achieve the most accurate estimation, on condition that the method is not out-of-time[4]. *ProbeSim, PRSim, and PRSim-IF* all use an absolute error parameter ε for single-source queries. We set $\varepsilon \in \{0.1, 0.05, 0.01, 0.005, ...\}$, where $\varepsilon = 0.1$ is the typical setting for *ProbeSim* as in [24], and $\varepsilon = 0.01$ is the typical setting for *PRSim* and *PRSim-IF*. For *TopSim*, since the baseline algorithm is extremely slow and has inferior answer quality, we use *Prio-TopSim*, the optimized algorithm for evaluation. We vary T , the depth of the traversal from 3 to 6 with default value as 3, and H, the size of priority pool from $1,000$ to $4,000$ with default value as $1,000$. *TSF* has two parameters R_g and R_q, which denotes the number of indexed one-way graphs and the number of times each one-way graph is reused in the query stage, respectively. We set $(R_g, R_q) \in \{(100, 20), (300, 40), (600, 80), (900, 120)\}$, where $(100, 20)$ is the default value. When the size of the index exceeds the memory capacity, we use its external memory version, i.e., *EXT-TSF*, which may incur longer query time for disk I/O. For *READS*, we vary parameter r, the number of indexes (i.e. SA forests) constructed during preprocessing, and rq, the number of random walks generated for each index at query time. Specifically, we set $(r, rq) \in \{(100, 10), (500, 10), (500, 20), (1000, 20)\}$ while by default $(r, rq) = (100, 10)$. For our algorithms, we set $\varepsilon_{min} = 10^{-6}$. The failure probability is set to 0.0001 for all sampling-based algorithms. Since all baselines under the typical parameter settings give significantly inferior performance compared to their precise parameter settings, we omit them in Fig. 5-8. More details can be referred to the full version of the paper [1].

We adopt the idea of *pooling* [24] to evaluate the relative effectiveness of different algorithms. We take *MC* as the ground truth for each candidate in the pool and guarantee that the estimation error is below 10^{-6} with confidence over 99.999%.

6.2 Evaluation of Top-k Queries

Metrics. We use Precision@k to evaluate the accuracy of top-k queries. Given a query node u, denote by V_k the set of top-k nodes with the largest SimRank values, and V'_k the estimated node set of a specific algorithm. The metric is defined as $Precision@k = \frac{|V_k \cap V'_k|}{k}$. In the evaluation, we varying k in $\{1, 5, 10, 50, 100, 500, 1000\}$. Intuitively, as k increases, the problem incurs higher computational cost because the top-k answers are harder to be distinguished from other nodes.

Our query results are illustrated in Fig. 5 & 6. Generally speaking, all baselines achieve better performance for the medium values of k, while the precision decreases as k goes towards 1 or $1,000$. In particular, the two algorithms that adopt random walk sampling in both the forward and backward stage, i.e., *TSF* and *READS*, achieve the highest query speed with the help of index, but give significantly inferior query accuracy compared to other baselines. This is attributed to that the number of indices constructed are determined heuristically, partially because of the tremendous time and space overhead. Hence, the estimation error can not be guaranteed in practice. Methods with graph-traversal based searching strategies, including *TopSim*, *ProbeSim*, *PRSim*, and *PRSim-IF*, incur much higher query cost but achieve relatively satisfying accuracy. *TopSim* acquires surprisingly good performance in terms of Precision@k, since intuitively the most similar nodes locate close to the query node. Overall, *PRSim-IF* and *PRSim* are the two best baseline algorithms with a good tradeoff between query accuracy, computational cost, and index size (for *PRSim*). In comparison, the precision of *SimTab-Top-k* is always 1 in our experiments. This is achieved by our multi-armed bandit modeling of the problem, which enables us to treat the nodes adaptively in the sampling process. Meanwhile, our algorithm is orders of magnitude faster than those baselines with acceptable query accuracy, e.g, *PRSim-IF*. Note that the precision of these algorithms still have a gap from 1, and remain non-stable for different datasets and k. On the other hand, the answer quality can hardly be improved, because these algorithms cannot efficiently query with smaller parameters for the tremendous time and index cost. Lastly, the query time of *SimTab-Top-k* varies with k, which implies that our algorithm is adaptive to the hardness of the queries.

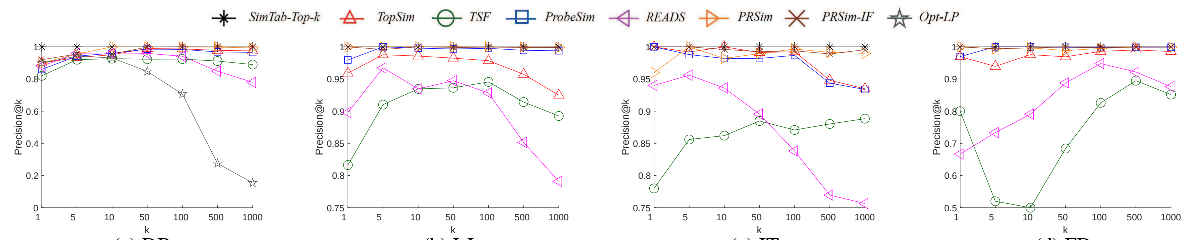
To demonstrate the uniqueness and hardness of the top-k query, we also compare with *Opt-LP*, the state-of-the-art all-pair SimRank algorithm, which is also the most scalable one for large graphs. Following [31], we set the absolute error parameter ε to 0.01. Unfortunately, even under such a loose parameter setting, *Opt-LP* can only compute the SimRank similarities on DB, the smallest dataset, and fails on three other datasets due to out of memory. Besides, the query accuracy in terms of Precision@k is inferior to all compared single-source algorithms. This indicates that the top-k SimRank query cannot be easily answered via direct SimRank computation and should be specially considered.

6.3 Evaluation of Thresholding Queries

Metrics. For the thresholding query, we vary $\tau \in \{10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}\}$. We use precision, recall and F1-score as the evaluation metrics. Specifically, let S be the set of exact answers for thresholding queries, and S' the node set returned by some specific algorithm. We define $Precision = \frac{|S \cap S'|}{|S'|}$, $Recall = \frac{|S \cap S'|}{|S|}$, and $F1-score = 2 \cdot \frac{Precision \cdot Recall}{Precision + Recall}$.

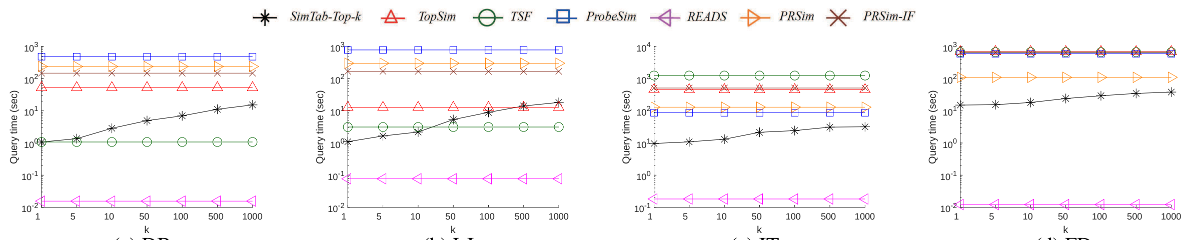
The query results are demonstrated in Fig. 7 & 8. For space constraints, we only show F1-Score in Figure 7. The following conclusions are easily derived. First, the query is harder for smaller τ. Since most nodes have low SimRank values w.r.t. the query node, more nodes need to be estimated precisely for smaller τ. Consequently, the F1-score of baseline algorithms decreases as τ shrinks. Second, at the cost of longer query time, *PRSim-*

[4]We say an algorithm is out-of-time if the query time for some node is over one hour or the index construction time is beyond 10,000 seconds. This indicates that the algorithm is not suitable for dynamic graphs.



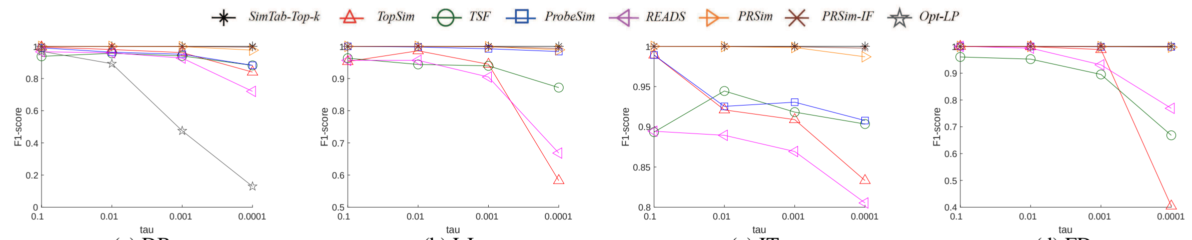
(a) DB (b) LJ (c) IT (d) FD

Figure 5: Precision@k for top-k queries, varying $k \in \{1, 5, 10, 50, 100, 500, 1000\}$



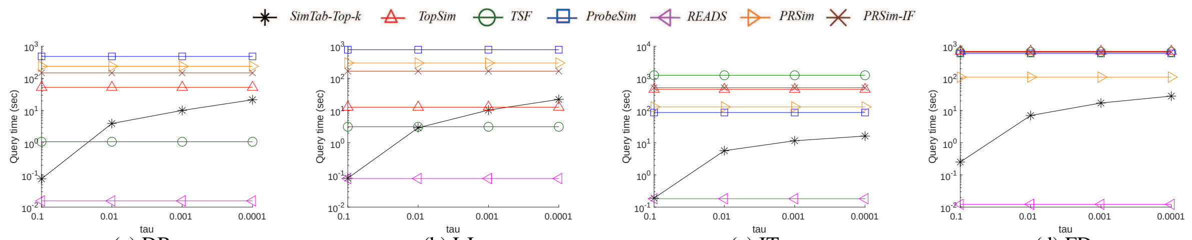
(a) DB (b) LJ (c) IT (d) FD

Figure 6: Query time for top-k queries, varying $k \in \{1, 5, 10, 50, 100, 500, 1000\}$



(a) DB (b) LJ (c) IT (d) FD

Figure 7: F1-score for thresholding queries, varying $\tau \in \{10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}\}$



(a) DB (b) LJ (c) IT (d) FD

Figure 8: Query time for thresholding queries, varying $\tau \in \{10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}\}$

IF achieves the best performance among all index-free baselines with F1-score close to 1, while *PRSim* is the best index-free algorithm. As Fig. 7 shows, *TopSim* is not suitable for thresholding queries especially for small τ, because a large fraction of the answer is missed due to the truncated search and the heuristic pruning rule. Similar to the top-k query, the answer quality of *TSF* and *READS* is significantly inferior to those algorithms with graph-traversal based strategies, such as *PRSim-IF* and *PRSim*. Therefore, they should not be recommended to answer these queries. Again, our *SimTab-Thres* algorithm enables to answer all queries exactly, with query efficiency significantly outperforming any baseline that achieves acceptable answer quality.

7. CONCLUSIONS

In this paper, we propose algorithms to improve both the efficiency and the effectiveness of the state-of-the-art methods over top-k and thresholding SimRank queries. Specifically, we integrate several techniques to tighten the confidence bounds of SimRank estimation, including the empirical Bernstein inequality, variance reduction tricks, and careful algorithm design. Moreover, we model the top-k and thresholding SimRank queries as the multi-armed bandits problems, so that the algorithm complexity is determined by the hardness of the query instance. By proposing novel arm sampling strategies, we are able to significantly enhance the practical efficiency of the algorithms. We conduct extensive experiments for top-k and thresholding queries on large-scale graphs, and the results indicate that our algorithms are the only acceptable methods to achieve stable and satisfying performance in terms of answer quality and with reasonable query efficiency.

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Algorithm 7: EBSim: The Single-Pair SimRank Algorithm

```
Input: Directed graph $G = (V, E)$; $u, v \in V$; Error $\varepsilon$ and
       failure probability $\delta$
Output: $\hat{s}(u, v)$, the estimation for the SimRank $s(u, v)$
1  $X \leftarrow 0, t \leftarrow 1$ ;
2  while $\sqrt{2X \ln \frac{3 \ln^2 t}{\delta}} + 3 \ln \frac{3 \ln^2 t}{\delta} \geq \varepsilon t$ do
3      for $s = 1$ to $t$ do
4          $x \leftarrow u, y \leftarrow v$;
5          while $rand() \leq c$ do
6              $x \leftarrow rand(I(x))$ and $y \leftarrow rand(I(y))$;
7              if $x = y$ then
8                  $X \leftarrow X + 1$;
9                  Break;
10     $t \leftarrow 2 * t$;
11 return $\hat{s}(u, v) = X/t$;
```

9. APPENDIX

9.1 Approximate Queries

9.1.1 Approximate top-k queries

SimTab-Top-k is able to answer the approximate top-k SimRank query with a slight modification of the algorithm. We first give the formal definition as below.

DEFINITION 6 (APPROXIMATE TOP-k QUERIES). *We are given a node u in G, a positive integer $k < n$, a precision guarantee p, and a failure probability δ, and let V_k be the set of nodes in G whose SimRank similarity to u is the top-k largest, with a small error tolerance parameter ε_{min} (e.g., 10^{-6}). In particular, let v_k be the node with the k-th largest SimRank value w.r.t. the query node u, we have $V_k = \{v|s(u, v) \geq s(u, v_k) - \varepsilon_{min}\}$. An approximate top-$k$ SimRank query returns a set of k nodes V'_k, such that $|V'_k \cap V_k| \geq pk$.*

To answer the approximate version of the top-k query, our prefiltering algorithm is modified as follows. In each iteration i, after we compute an estimation $\hat{s}(u, v)$ (and $\beta(v)$) for each v, we find the node v' with the $\lceil p'k \rceil$-th largest lower bound, and use it to select the candidate set. This guarantees that at least $\lceil p'k \rceil$ actual top-k answers are included in the candidates. Note that any choice of $p' \in [p, 1]$ is sufficient; for example, we can set $p' = \frac{p+1}{2}$. For the top-k identification phase, in each iteration, instead of finding V_k, the top-k nodes with the smallest $B(v)$, we compute $V_{\lceil pk \rceil}$, which only contains the top-$\lceil pk \rceil$ nodes. Intuitively, since the distribution of SimRank values approximately follows the power law, the gap between the $\lceil pk \rceil$-th and the $(\lceil pk \rceil + 1)$-th SimRank value is larger than that between the k-th and the $(k + 1)$-th SimRank. Hence, the stopping conditions are relaxed, and the approximate algorithm should terminate earlier than the exact one.

9.1.2 Approximate thresholding queries

Our algorithm can be easily extended to answer the approximate thresholding query, which is defined as follows.

DEFINITION 7 (APPROXIMATE THRESHOLDING QUERIES). *We are given a node u in G, a real number $\tau \in [0, 1]$, a failure probability δ, and the approximation bound $p, r \in (0, 1)$ for precision and recall, respectively. An approximate thresholding SimRank query returns a set of nodes, denoted as V_τ, such that with $1 - \delta$ probability, $\frac{|V_\tau \cap S|}{|V_\tau|} \geq p$, $\frac{|V_\tau \cap S|}{|S|} \geq r$. Here, we denote by S the exact answer for the thresholding query, and with a small error tolerance parameter ε_{min} (e.g., 10^{-6}). In particular, we have $S = \{v|s(u, v) \geq \tau - \varepsilon_{min}\}$.*

The approximate algorithm only has slight differences with the exact version. Firstly, note that in each iteration of the prefiltering phase, a subset of the candidate C can be directly added to V_τ according to the pruning rule. We denote by the set of remained candidates as C', which will be returned after the prefiltering phase, and will be checked during the refinement phase. We assign a parameter $r' \in [r, 1]$ as the recall in the prefiltering phase. Once $\frac{|V_\tau|}{|V_\tau \cup C'|} \geq r'$, the prefiltering algorithm terminates. Also note that the precision is always 1 for the prefiltering phase, because of the correctness of the pruning rule, and the fact that adding false answer to the result cannot improve the efficiency of the algorithm.

Secondly, in the refinement phase, we have two choices on the stopping condition and the the returned set of nodes:
(1) The stopping condition is changed to $\frac{|V_\tau|}{|V_\tau \cup C'|} \geq r$. Return all nodes in V_τ. This guarantees the answer has precision 1 and recall at least $\frac{|V_\tau|}{|V_\tau \cup C'|}$.

(2) The stopping condition is changed to $\frac{|V_\tau|}{|V_\tau \cup C'|} \geq \max\{p, r\}$. Then, we return all nodes in V_τ and the nodes in C' with empirical mean above τ. In practice, since the confidence interval computed by any concentration inequality is a loose upper bound of the actual one, choice (2) usually achieves a higher F1-score than choice (1).

9.1.3 SimTab-Single: The algorithm for approximate single-pair queries

In this section, we show that how to use the empirical Bernstein inequality to speed up approximate single-pair SimRank queries. Previous work such as the Monte Carlo method employs Chernoff-Hoeffding inequality to bound the estimated error between the empirical and the true means. Comparing to the Chernoff-Hoeffding inequality, the empirical Bernstein inequality takes the empirical variance into consideration, and is proven to be tighter when the esitimation is close to 0. To be precise, if the SimRank value $s(u, v)$ is close to zero, the empirical variance of the estimator by random walk sampling is very small. Therefore, the confidence bound is approximately in reverse proportional to the sample size t, and is significantly tighter than the bound based on Chernoff-Hoeffding inequality which is in reverse proportional to $\sqrt{t}$. This suggests that algorithms based on the empirical Bernstein inequality requires fewer samples given an error threshold ε.

Our algorithm proceeds as follows (Algorithm 7). We start by setting the empirical sum X to be 0, and the number of samples t to be 1 (Line 1). For each iteration, we check if the stopping rule is satisfied (Line 2). If not, we take t more samples and double the value of t. Each sample is taken as follow. We set x to be u and y to be v (Line 4). On each step, we terminate the random walks with probability $1 - c$. With the remaining probability c, the two random walks proceed to an in-neighour of x and an in-neighour of y uniformly at random (Line 6). If the two random walks meet (Line 7), we increase the value of X by 1 and stop the random walks (Lines 8-9). Otherwise, the random walks proceed to the next step. When the stopping rule is satisfied, the algorithm stops and output $\hat{s}(u, v) = X/t$ as the estimation (Line 11).

To set the proper stopping time for single-pair algorithm, we need to make sure that when the algorithm stops, the condition

$|\hat{s}(u,v) - s(u,v)| < \varepsilon$ holds with probability $1-\delta$. Let t be the smallest t such that

$$\sqrt{2X \ln \frac{3\ln^2 t}{\delta}} + 3\ln\frac{3\ln^2 t}{\delta} \le \varepsilon t.$$

In particular, we have the following Lemma.

THEOREM 4. *With probability* $1-\delta$*, Algorithm 7 outputs* $\hat{s}(u,v) = X/t$ *such that* $|\hat{s}(u,v) - s(u,v)| < \varepsilon$.

PROOF. Please refer to Section 9.2. □

Next, we analyze the time complexity of *EBSim* with the following theorem.

THEOREM 5. *The EBSim algorithm runs in* $O(\frac{1}{\varepsilon} + \frac{s(u,v)}{\varepsilon^2}\log\frac{1}{\delta})$ *time in expectation.*

PROOF. Please refer to Section 9.2. □

9.2 Additional Lemmas, Theorems, and Proofs

PROOF OF LEMMA 3 (SKETCH). Recall that the *Sample-all-arms* algorithm estimates the SimRank values following Equation 6. First, for each $w \in V$ and each level $l \in [0, \infty)$, let $I_f(w,l)$ be the indicator variable such that $I_f(w,l) = 1$ if the walk $W(u)$ stops at w with exact l steps. According to the definition of $\pi_l(u,w)$, it is easy to see that

$$I_f(w,l) = \begin{cases} 1, & \text{with probability } \pi_l(u,w), \\ 0, & \text{otherwise.} \end{cases}$$

Hence, we have $\mathrm{E}[I_f(w,l)] = \pi_l(u,w)$ for each w and l. Second, let $I_d(w)$ be the indicating function such that $I_d(w) = 1$ if the two sampled $\sqrt{c}$-walks $W_1(w)$ and $W_2(w)$ do not meet. According to the definition of $d(w)$ [30], we have

$$I_d(w) = \begin{cases} 1, & \text{with probability } d(w), \\ 0, & \text{otherwise.} \end{cases}$$

It follows that $\mathrm{E}[I_d(w)] = d(w)$ for every w. Third, we prove that given w_l, the returned value $Score(u,v)$ is an unbiased estimator of $\frac{\pi_l(v,w_l)}{(1-\sqrt{c})^2}$ for each $v \in V \backslash \{u\}$. This is equivalent to that v is in H_{l-1} with probability $\pi_l(v,w_l)$, which can be proved by induction on the iterator j in Algorithm 3. Finally, note that the estimation $\hat{s}(u,v)$ can be written as

$$\hat{s}(u,v) = \sum_{w\in V}\sum_{l=0}^{\infty} I_f(w,l) I_d(w) Score(u,v).$$

We have

$$\begin{aligned}\mathrm{E}[\hat{s}(u,v)] &= \sum_{w\in V}\sum_{l=0}^{\infty} \mathrm{E}[I_f(w,l)]\mathrm{E}[I_d(w)]\mathrm{E}[Score(u,v)] \\ &= \frac{1}{(1-\sqrt{c})^2}\sum_{l=0}^{\infty}\sum_{w\in V}\pi_l(u,w)\pi_l(v,w)d(w) \\ &= s(u,v),\end{aligned}$$

and the lemma holds. □

PROOF OF THEOREM 1 (SKETCH). According to Lemma 3 and the empirical Bernstein inequality (Lemma 2), with at least $1-\delta$ probability, it holds that $s(u,v) \in [\hat{s}(u,v) - \beta(v), \hat{s}(u,v) + \beta(v)]$ for each $v \in V\backslash\{u\}$. We first prove the correctness of the pruning rule. Let v' be the node with the k-th largest lower bound. For some node v, if $\hat{s}(u,v') - \beta(v') + \varepsilon_{min} > \hat{s}(u,v) + \beta(v)$, we have $\min_{v'\in C} s(u,v') + \varepsilon_{min} > s(u,v)$, i.e., the k nodes in the candidate set C are at least as good as v by up to error ε_{min}. Therefore, v can be safely pruned, and the returned candidate C will contain at least k nodes in the right answer. □

PROOF OF LEMMA 4 (SKETCH). Note that Algorithm 4 is an implementation of the UGapEc algorithm in [12]. According to Theorem 2 of [12], the time complexity is bounded by $H_{k,\varepsilon_{min}}\log\frac{H_{k,\varepsilon_{min}}}{\delta}$. Recall our setting of $\varepsilon_{min} = 10^{-6}$, we have $\log H_{k,\varepsilon_{min}} \le \log\frac{n}{\varepsilon_{min}{}^2} \sim \log n$.

Next, we prove that the addition of the *sample-all-arms* strategy indeed improves the algorithm complexity. Note that the Top-k-Identification algorithm is only invoked when applying sample-one-arm strategy to each candidate is more efficient than applying the sample-all-arms strategy. In ohter words, the inequation $|C|t_o \le t_a$ holds (Line 11 of Algorithm 2). Since there exists at most $\frac{t_a}{t_o}$ candidates, the complexity of the top-k identification phase can be formalized as

$$\max_{\substack{|S|=t_a/t_o,\\ S\subseteq V}} \sum_{v\in S}\frac{1}{\max{(\Delta_v, \varepsilon_{min})}^2}\log\frac{n}{\delta}.$$

Let $\theta = \frac{t_a}{t_o}$. It is clear that the above complexity can be bounded by

$$\min{(\frac{\theta}{\varepsilon_{min}{}^2}\log\frac{n}{\delta}, \sum_{v\in V\backslash\{u\}}\frac{1}{\max{(\frac{\Delta_v+\varepsilon_{min}}{2}, \varepsilon_{min})}^2}\log\frac{n}{\delta})}.$$

□

PROOF OF THEOREM 2 (SKETCH). The correctness of the *SimTab-Top-k* algorithm can be derived from the correctness of the *Prefiltering* algorithm (Theorem 1) and the *Top-k-Identification* algorithm (Lemma 4). For both phases, we set the failure probability as $\frac{\delta}{2}$. By union bound, the failure probability of Lemma 4 is at most δ.

Now we need to prove that, when *SimTab-Top-k* terminates at the prefiltering phase (Lines 13-15 of Algorithm 2) and does not proceed to the top-k identification phase, the algorithm complexity is still bounded by

$$\min{(\frac{\theta}{\varepsilon_{min}{}^2}\log\frac{n}{\delta}, \sum_{v\in V\backslash\{u\}}\frac{1}{\max{(\frac{\Delta_v+\varepsilon_{min}}{2}, \varepsilon_{min})}^2}\log\frac{n}{\delta})}.$$

First, recall that t_a denotes the running time of one sample-all-arms operation, while t_o denotes the running time of one sample-one-arm operation. Since sample-one-arm is implemented by sampling a coupled random walk, the expected time complexity is $O(1)$ for the walks have constant expected length. Therefore, $\theta = \frac{t_a}{t_o}$ denotes the time complexity of one sample-all-arms operation. When the algorithm terminates at the prefiltering phase, it satisfies that $|C|t_o > t_a$, i.e., $\theta < |C| \le n$. In practice, due to the skewed distribution of SimRank values, θ is much smaller than n in most cases.

Second, according to the Chernoff-Hoeffding inequality, by invoking sample-all-arms $O(\frac{1}{\varepsilon_{min}{}^2}\log\frac{n}{\delta})$ times, we guarantee that the absolute error of each estimation $\hat{s}(u,v)$ is bounded by ε_{min}, with $O(\frac{\theta}{\varepsilon_{min}{}^2}\log\frac{n}{\delta})$ time cost. Indeed, this is a rather loose analysis, and the complexity may be improved via more tight concentration inequalities.

Finally, note that in this case, the time complexity of the top-k identification phase is asymptotically higher than the prefiltering phase, i.e., $O(\frac{\theta}{\varepsilon_{min}{}^2}\log\frac{n}{\delta}) = \min{(\frac{\theta}{\varepsilon_{min}{}^2}\log\frac{n}{\delta}, \sum_{v\in V\backslash\{u\}}\frac{1}{\max{(\frac{\Delta_v+\varepsilon_{min}}{2}, \varepsilon_{min})}^2}\log\frac{n}{\delta})}$. This completes our proof. □

PROOF OF LEMMA 5 (SKETCH). Time complexity. According to [5], the time complexity of forward push is bounded by $O(\frac{1}{r_{max}})$. Note that for each candidate v, we set $r_{max}(v) = \frac{1}{n_r(v)}$, where $n_r(v)$ is the number of walks already sampled from v. Hence, the time cost of the push operation is asymptotically identical to the cost of walk sampling, i.e., $O(n_r(v))$. For the query node u, by setting $n_r(u) = \sum_{v \in C} n_r(v)$, the cost of forward push can also be bounded while providing a more accurate estimation.

Space complexity. Note that the cost of storing SimRank estimation for all nodes is $O(n)$. On the other hand, each node need extra $O(1)$ space cost for the data structures of the push operation. Therefore, the asymptotic space complexity is the same as that of Algorithm 4. $\square$

PROOF OF THEOREM **??** (SKETCH). By [26], the time complexity of the thresholding bandit algorithm (i.e., *APT*) under the fixed confidence setting is $O(\sum\limits_{v \in V \setminus \{u\}} \frac{1}{(\Delta_{\mathcal{T},v}+\varepsilon_{min})^2} \log\frac{n}{\delta}))$. With a similar analysis in the proof of Lemma 4 and Theorem 2, the time complexity can also be improved by the sample-all-arms strategy, which results in an complexity of $\min(O(\frac{\theta}{\varepsilon_{min}{}^2}\log\frac{n}{\delta}), O(\sum\limits_{v \in V \setminus \{u\}} \frac{1}{(\Delta_{\mathcal{T},v}+\varepsilon_{min})^2} \log\frac{n}{\delta}))$. $\square$

PROOF OF THEOREM 4. Note that the algorithm can only stop at $t = 2^i$ for $i = 0, 1, 2, \ldots$ Let $\mathcal{E}_i$ denote the event that the algorithm stops at $t = 2^i$, but gives wrong estimation, i.e., $|\hat{s}(u,v) - s(u,v)| \geq \varepsilon$. Since Algorithm 7 stops if and only if

$$\sqrt{2X \ln \frac{3\ln^2 t}{\delta}} + 3 \ln \frac{3 \ln^2 t}{\delta} < \varepsilon t,$$

it follows that

$$\sqrt{\frac{X}{t} \cdot \frac{2 \ln \frac{3\ln^2 t}{\delta}}{t}} + \frac{3 \ln \frac{3\ln^2 t}{\delta}}{t} < \varepsilon.$$

Note that

$$X = \sum_{i=1}^{t} X_i = \sum_{i=1}^{t} X_i^2 \geq \sum_{i}^{t} (X_i - X/t)^2 = \bar{\sigma}_t^2,$$

Thus, we have

$$\bar{\sigma}_t^2 \cdot \sqrt{\cdot \frac{2 \ln \frac{3\ln^2 t}{\delta}}{t}} + \frac{3 \ln \frac{3\ln^2 t}{\delta}}{t} < \varepsilon.$$

By Lemma 2, it follows that with probability $1 - \frac{\delta}{\ln^2 t}$,

$$\Pr[\mathcal{E}_i] = \Pr[|\hat{s}(u,v) - s(u,v)| \geq \varepsilon] \leq \frac{\delta}{\ln^2 t} = \frac{\delta}{\ln^2 2^i} = \frac{1}{i^2} \cdot \frac{\delta}{\ln^2 2}.$$

By union bound, the probability that none of $\mathcal{E}_1, \mathcal{E}_2, \ldots, \ldots$ happens is bounded by

$$1 - \sum_{i=1}^{\infty} \Pr[\mathcal{E}_i] \geq 1 - \sum_{i=1}^{\infty} \frac{1}{i^2} \cdot \frac{\delta}{\ln^2 2} \geq 1 - \delta.$$

This proves that when Algorithm 7 stops, it outputs $\hat{s}(u,v) = X/t$ such that with probability $1 - \delta$, $|\hat{s}(u,v) - s(u,v)| < \varepsilon$. $\square$

PROOF OF THEOREM 5. First note that for reasonable setting of δ (e.g., $\delta = \frac{1}{n}$), when $t = \Theta(\frac{1}{\varepsilon})$ it satisfies that

$$3 \ln \frac{3 \ln^2 t}{\delta} \leq \varepsilon t/2.$$

Therefore, the probability that the algorithm does not stop at t is at most

$$\Pr\left[\sqrt{2X \ln \frac{3\ln^2 t}{\delta}} > \frac{\varepsilon t}{2}\right].$$

We bound the probability for $t_i = O(2^i \cdot \frac{s(u,v)}{\varepsilon^2} \log\frac{1}{\delta}))$ for $i = 1, 2, \ldots$, repsectively. Note that the theorem holds if $t \leq \frac{s(u,v)}{\varepsilon^2} \log \frac{1}{\delta}$. Since

$$\Pr\left[\sqrt{2X \ln \frac{3\ln^2 t}{\delta}} > \frac{\varepsilon t}{2}\right] = \Pr\left[2X \ln \frac{3\ln^2 t}{\delta} > \frac{\varepsilon^2 t^2}{4}\right] = \Pr\left[\frac{X}{t} > \frac{\varepsilon^2 t}{8 \ln \frac{3 \ln^2 t}{\delta}}\right],$$

when $t = t_i = \frac{2^i \cdot s(u,v)}{\varepsilon^2} \log \frac{1}{\delta}$, the probability is

$$\Pr\left[\frac{X}{t} > s(u,v) \cdot \frac{2^i \log \frac{1}{\delta}}{8 \ln \frac{3\ln^2 t}{\delta}}\right].$$

It can be proved that for reasonable setting of δ, $\frac{\log\frac{1}{\delta}}{8 \ln \frac{3\ln^2 t}{\delta}} > \frac{1}{64}$ for all i and $s(u,v) \in [0,1]$. By Markov's inequality,

$$\Pr\left[\frac{X}{t} > s(u,v) \cdot \frac{2^i}{64}\right] \leq \frac{64}{2^i}.$$

Therefore, for any $t = t_i$, we have $t \Pr\left[\sqrt{2X \ln \frac{3 \ln^2 t}{\delta}} > \frac{\varepsilon t}{2}\right] \leq \frac{64 s(u,v)}{\varepsilon^2} \log \frac{1}{\delta}$. Also note that $t = t_i$ and $t = t_j$ are mutually exclusive for $i \neq j$. Hence the expected running time of Algorithm 7 is bounded by $O(\frac{1}{\varepsilon} + \frac{s(u,v)}{\varepsilon^2} \log \frac{1}{\delta})$. $\square$

Table 7: Query time of each baseline algorithm on LJ.

Method	Parameters	Query time	Index Time	Index size
TopSim	T: $(3, 1000)$	12.78	N/A	N/A
	P: same as T	N/A	N/A	N/A
TSF	T: $(100, 20)$	0.068	24.03	3.61
	P: $(900, 120)$	3.14	186.3	32.52
ProbeSim	T: 0.1	0.042	N/A	N/A
	P: 0.0005	781.22	N/A	N/A
READS	T: $(100, 10)$	0.041	246.04	2.9
	P: $(1000, 20)$	0.077	1176.05	19.15
PRSim	T: 0.01	0.54	13.68	0.1
	P: 0.0005	301.46	237.59	1.56
PRSim-IF	T: 0.01	1.15	N/A	N/A
	P: 0.001	168.23	N/A	N/A
Opt-LP	T: 0.01	N/A	N/A	Out-of-memory

9.3 More Experiments

This section demonstrates the additional experimental results for both top-k and thresholding SimRank queries.

9.3.1 Experimental results for randomly generated queries

Table 6: Query time of each baseline algorithm on DB, with both the typical parameter setting (denoted as T) and the precise parameter setting (denoted as P). Query time and index time are measured in seconds, while index size is measured in gigabytes (GB).

Method	Parameters	Query time	Index Time	Index size
TopSim	T: $(3, 1000)$	0.044	N/A	N/A
	P: $(6, 4000)$	52.71	N/A	N/A
TSF	T: $(100, 20)$	0.038	28.58	4.04
	P: $(900, 120)$	1.07	281.14	36.39
ProbeSim	T: 0.1	0.0045	N/A	N/A
	P: 0.0001	482.28	N/A	N/A
READS	T: $(100, 10)$	0.012	206.05	2.65
	P: $(1000, 20)$	0.016	1826.05	20.85
PRSim	T: 0.01	0.5	8.87	0.31
	P: 0.0005	238.51	82.05	2.52
PRSim-IF	T: 0.01	1.19	N/A	N/A
	P: 0.001	148.37	N/A	N/A
Opt-LP	T: 0.01	N/A	1324.88	75.3

Tables 6-9 list the query time of all baseline single-source and all-pair algorithms for DB, LJ, IT, and FD, respectively. Specifically, for each single-source algorithm, we report both the typical and precise parameter settings and the corresponding query time, index time (if applicable) and index size (if applicable). Note that the typical parameter setting follows the original paper, while the precise parameter setting is the one among our parameter settings that achieves the most accurate estimation and stays away from out-of-time. Typically, the precise parameter setting means more indices are constructed for the index-based algorithm, or smaller absolute error guarantee for the sampling-based algorithm. For the compared all-pair SimRank algorithm, we only conduct experiments under the typical parameter setting, where the error parameter ε is set to 0.01 as in [31]. This is because the algorithm needs excessive memory space, which make it infeasible for large graphs or with smaller parameter settings, as shown by our experiment.

The conclusions are as follows. First, for any baseline algorithm, the query costs under typical and precise parameter settings have a large difference. Generally speaking, the query time under the precise parameter setting is about 3-5 orders of magnitude slower than that under the typical parameter setting, except for *TSF* and *READS*. For these two methods, the query time is in proportional to the number of indices constructed and the time each index is reused. However, the algorithm under the precise parameter setting takes significantly longer time for index construction, and the index needs more memory (or disk) space. Consequently, these algorithms can not scale to large graphs with accurate parameter settings. Moreover, to reduce the space and time cost for building the index, the parameters are selected heuristically. For example, although theoretically *READS* has absolute error guarantee, the selection of parameters make it a heuristic algorithm to avoid excessive index size. As the experiment shows, this dramatically affects the query accuracy of the algorithm.

Secondly, the graph traversal based algorithms, including *TopSim*, *ProbeSim*, *PRSim*, and *PRSim-IF*, it is hard to get a good tradeoff between the query cost and the query accuracy. *TopSim* adopts similarity path enumeration in both the forward and backward searching stage, which makes it vulnerable to the local graph structure. For example, we speculate that LJ and FD are locally dense graphs [32], because *TopSim* fails with more precise parameters (i.e., longer searching steps). On the other hand, *ProbeSim*, *PRSim*, and *PRSim-IF* use random walk sampling in the forward searching stage, and achieve better scalability. Their query costs are approximately in proportion to $\frac{1}{\varepsilon^2}$ according to the theoretical analysis and our empirical evaluation. Nonetheless, they still can not answer the query with error parameter under $\varepsilon = 10^{-4}$.

At last, our empirical evaluation demonstrates that all-pair SimRank algorithms are not suitable for our studied queries. Even for the most scalable algorithm, *Opt-LP*, the memory cost (and possibly the computational cost) is too large so that it can not work well on a machine with 128GB memory. Also note that the query time is inapplicable for *Opt-LP*, since it can pre-compute all SimRank similarities and sort them in descending order for each node, and answer the top-k query (resp. the thresholding query) in $O(k)$ (resp. $O(\log n)$) time. However, this is achieved by sacrificing the efficiency of pre-computation and the query accuracy.

We demonstrate the query accuracy of each algorithm for the top-k queries (resp. the thresholding queries) with the typical parameter setting, in Figure 9 (resp. Figure 10). Compared to the

Table 8: Query time of each baseline algorithm on IT.

Method	Parameters	Query time	Index Time	Index size
TopSim	T: $(3, 1000)$	3.0	N/A	N/A
	P: $(5, 3000)$	455.56	N/A	N/A
TSF	T: $(100, 20)$	0.15	120.41	30.76
	P: $(600, 80)$	1248.86	1252.34	184.58
ProbeSim	T: 0.1	0.015	N/A	N/A
	P: 0.001	87.06	N/A	N/A
READS	T: $(100, 10)$	0.18	1364.51	30.38
	P: same as T	N/A	N/A	N/A
PRSim	T: 0.01	1.24	80.58	3.94
	P: 0.001	129.95	267.14	16.11
PRSim-IF	T: 0.01	5.08	N/A	N/A
	P: 0.001	511.73	N/A	N/A
Opt-LP	T: 0.01	N/A	N/A	Out-of-memory

Table 9: Query time of each baseline algorithm on FD.

Method	Parameters	Query time	Index Time	Index size
TopSim	T: $(3, 1000)$	693.95	N/A	N/A
	P: same as T	N/A	N/A	N/A
TSF	T: $(100, 20)$	0.3	945.7	50.92
	P: $(300, 40)$	667.72	1164.19	152.77
ProbeSim	T: 0.1	1.1	N/A	N/A
	P: 0.001	597.14	N/A	N/A
READS	T: $(100, 10)$	0.55	4919.55	58.19
	P: same as T	N/A	N/A	N/A
PRSim	T: 0.01	1.35	1282.08	0.46
	P: 0.001	110.0	7933.27	4.21
PRSim-IF	T: 0.01	1.21	N/A	N/A
	P: 0.0005	653.88	N/A	N/A
Opt-LP	T: 0.01	N/A	N/A	Out-of-memory

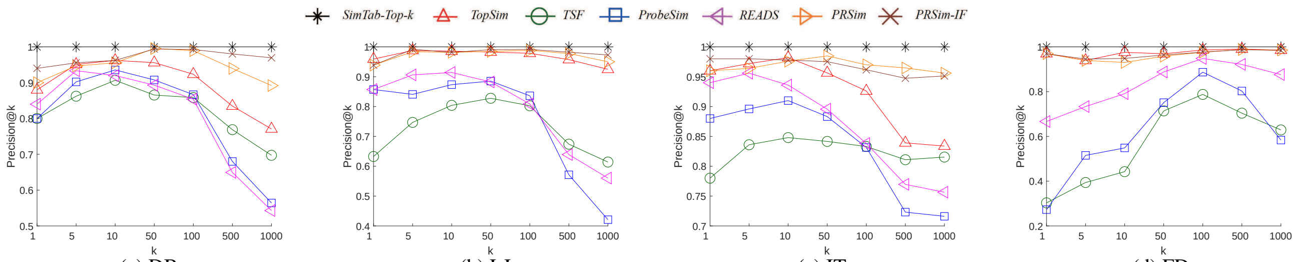
Table 11: Query time of *SimTab-Thres* on four datasets.

Dataset	$\tau = 0.1$	$\tau = 0.01$	$\tau = 0.001$	$\tau = 0.0001$
DB	0.075	3.97	10.12	21.7
LJ	0.079	2.92	10.35	22.3
IT	0.19	5.67	11.55	16.16
FD	0.25	7.04	17.21	28.21

precise parameter setting, the query accuracy decreases by a significant margin. Besides, the degeneration varies for different datasets. For DB and IT, the top-k query is harder (see *PRSim-IF*, the best baseline, as an example). For all datasets, the degeneration of the thresholding queries with small τ (e.g., 10^{-4}) is obvious, even for *PRSim* and *PRSim-IF*. We conclude that reducing the query cost by setting loose parameters is not a reasonable choice for the top-k and thresholding queries.

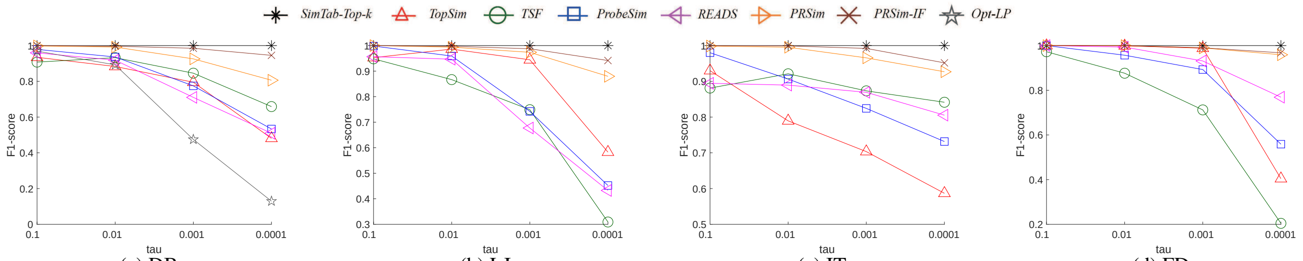
We also plot the precision and recall of the thresholding SimRank queries with the *precise* parameter setting in Figure 11 & 12, as a supplement to Figure 7. For precision, only *TSF* and *READS* give inferior results, while all other single-source baselines achieve a precision close to one. This mainly results from that the implementation of *TSF* and *READS* give no absolute error guarantee. Besides, it is harder for single-source algorithms to achieve high recall than precision. Some answers will be missed by allowing an error parameter for each estimation and treating them equally.

Table 10 & 11 show the query time of *SimTab-Top-k* and *SimTab-Thres* for all four datasets.



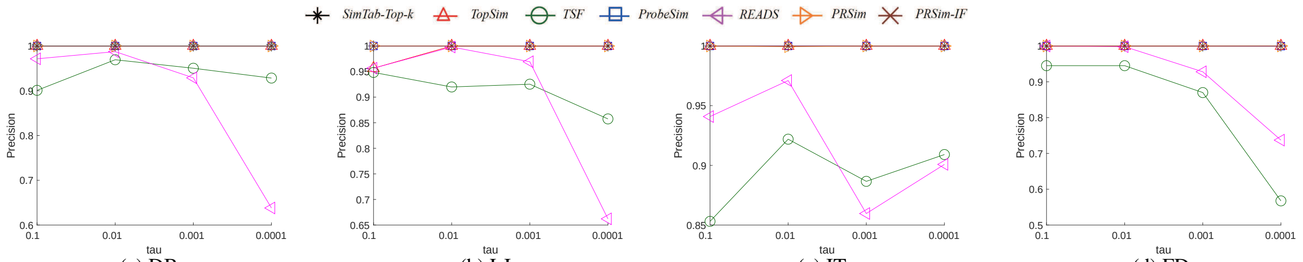
(a) DB (b) LJ (c) IT (d) FD

Figure 9: Precision@k of the top-k queries, varying $k \in \{1, 5, 10, 50, 100, 500, 1000\}$. All baselines are with their typical parameter settings.



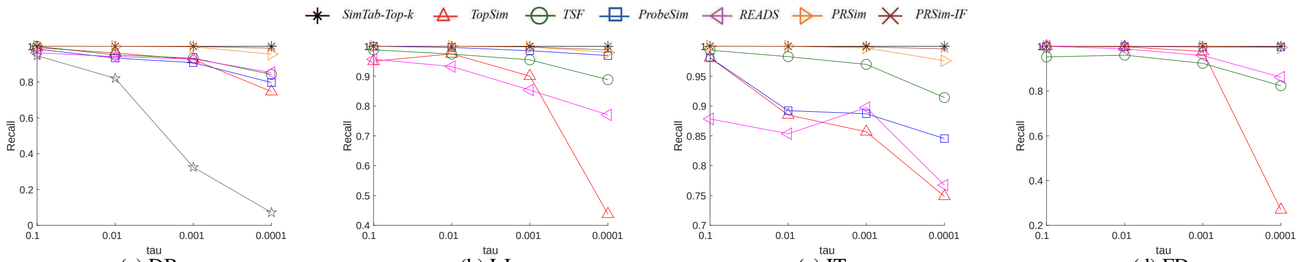
(a) DB (b) LJ (c) IT (d) FD

Figure 10: F1-score of the thresholding queries, varying $\tau \in \{0.1, 0.01, 0.001, 0.0001\}$. All baselines are with their typical parameter settings.



(a) DB (b) LJ (c) IT (d) FD

Figure 11: Precision of the thresholding queries, varying $\tau \in \{0.1, 0.01, 0.001, 0.0001\}$. All baselines are with their precise parameter settings.



(a) DB (b) LJ (c) IT (d) FD

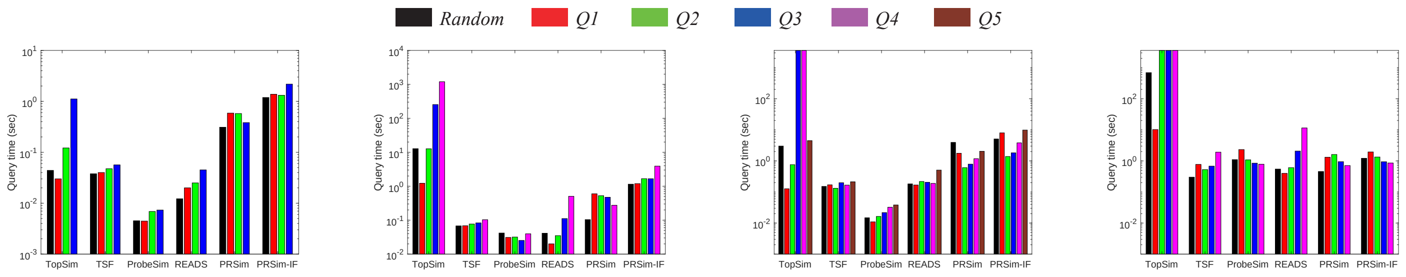
Figure 12: Recall of the thresholding queries, varying $\tau \in \{0.1, 0.01, 0.001, 0.0001\}$. All baselines are with their precise parameter settings.

9.3.2 Experimental results for queries using stratified sampling

In this section, all experimental results of the baseline algorithms, including query time and accuracy, are evaluated with their typical parameter settings. This is because for a specific algorithm and with different queries, the precise parameter setting may vary. (Note that the definition of the precise parameter setting is the choice of parameters that achieves the best possible query accuracy, on condition that the algorithm is not out-of-time.) Recall that we split the nodes by their in-degrees into intervals $[1, 10)$, $[10, 10^2)$, $[10^2, 10^3)$, $[10^3, 10^4)$ and $[10^4, \infty)$, where the query nodes are denoted as Q1, Q2, Q3, Q4, and Q5, respectively. In particular, some datasets do not have nodes with very high in-degrees. For example, although FD is the largest datasets used in the experiment, there does not exist any nodes of in-degree lager than 10^4. Figure 13 reports the query time of all single-source baseline algorithms for the queries generated via stratified sampling.

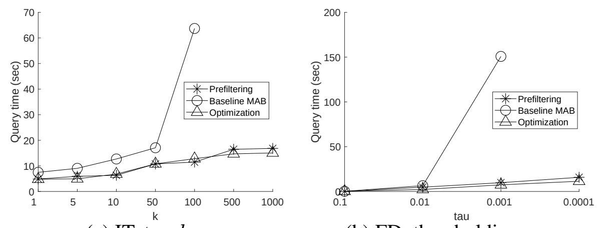
Table 10: Query time of *SimTab-Top-k* on four datasets.

Dataset	$k=1$	$k=5$	$k=10$	$k=50$	$k=100$	$k=500$	$k=1000$
DB	1.07	1.36	2.87	4.96	6.99	11.2	15.29
LJ	1.11	1.66	2.19	5.36	8.96	14.13	18.26
IT	9.66	10.87	13.13	21.55	24.29	31.18	34.89
FD	15.09	15.51	18.17	24.14	29.46	34.78	38.3



(a) DB (b) LJ (c) IT (d) FD

Figure 13: Time cost of baseline algorithms for queries using stratified sampling and with the typical parameter settings



(a) IT, top-k query (b) FD, thresholding query

Figure 24: An example of our optimization techniques over top-k and thresholding SimRank queries.

As Figure 13 shows, the query time of the baselines are only slightly affected by the query nodes, except for *TopSim*. Note that for *TSF* and *READS*, the number of indices constructed is predetermined and independent of the query node. For *ProbeSim*, *PRSim*. and *PRSim-IF*, they all firstly employ the random walk sampling in the forward searching stage. Secondly, for the graph traversal based backward stage, they either adopt index to reduce the query cost or use a randomized searching procedure, which also alleviate the tremendous overhead of the traversal. On the contrary, since *TopSim* uses BFS-based traversal in both searching stages, its query efficiency is largely influenced by the number of in-neighbors of the query node. For query nodes with large in-degrees on IT and FD, TopSim fails to give the SimRank estimation within 3,600 seconds. As a comparison, we list the query time of *SimTab-Top-k* and *SimTab-Thres* for different queries in Figure 14 and Figure 15, respectively. The query complexity of our algorithms are sensitive to the in-degree of the query node, because for nodes with higher in-degrees, the SimRank scores are smaller, and their distribution is more flat. Hence, it takes more time to find the precise results.

Figures 16 - 19 list Precision@k of the top-k SimRank queries on different query nodes. Generally speaking, the query accuracy declines as the in-degree of the query node increases. Among the compared algorithms, only *PRSim* and *PRSim-IF* have acceptable accuracy. Nevertheless, their performance on IT and FD with Q3-Q5 are still not good. Note that our algorithm is able to return the precise answers (with a small failure probability), at the cost of a little more time consumption on these queries.

We demonstrate the query performance in terms of F1-score for thresholding SimRank queries in Figure 20 - 23. Again, only *PRSim* and *PRSim-IF* give reasonable query accuracy, though they are also incapable of handling queries of large in-degrees and with small τ on some tested datasets.

9.3.3 Empirical analysis of the optimization techniques

Finally, we demonstrate an example in Fig. 24 for the effectiveness of our optimization techniques in answering top-k and thresholding SimRank queries. For each query, we plot the time cost of the prefiltering phase, the baseline MAB algorithm, and the optimized algorithm with all techniques to reduce the confidence bounds. As the Figure shows, a direct implementation of the MAB algorithm incurs prohibitive cost and fails on the hard query parameters. In contrast, the optimized solution achieves much higher efficiency, for tighter confidence bound effectively reduces the number of samples in practice.

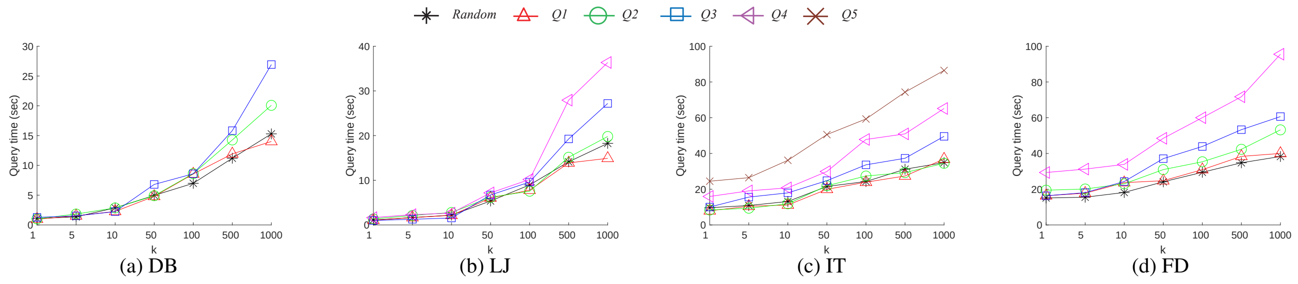


Figure 14: Time cost of our *SimTab-Top-k* algorithm for queries using stratified sampling

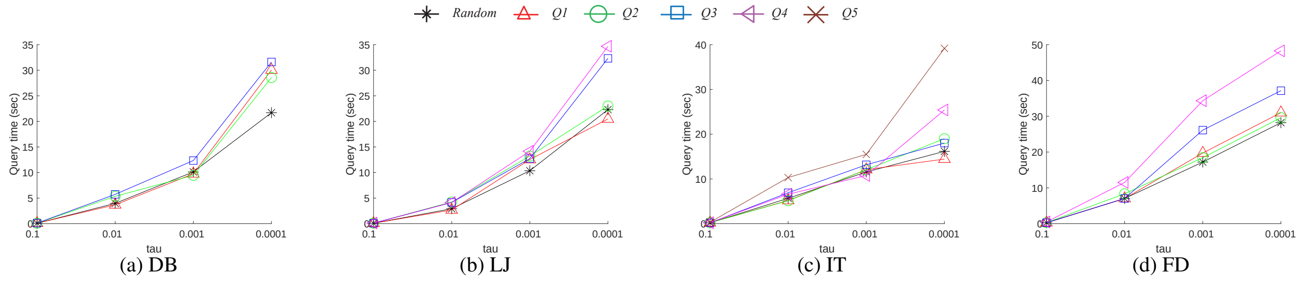


Figure 15: Time cost of our *SimTab-Thres* algorithm for queries using stratified sampling

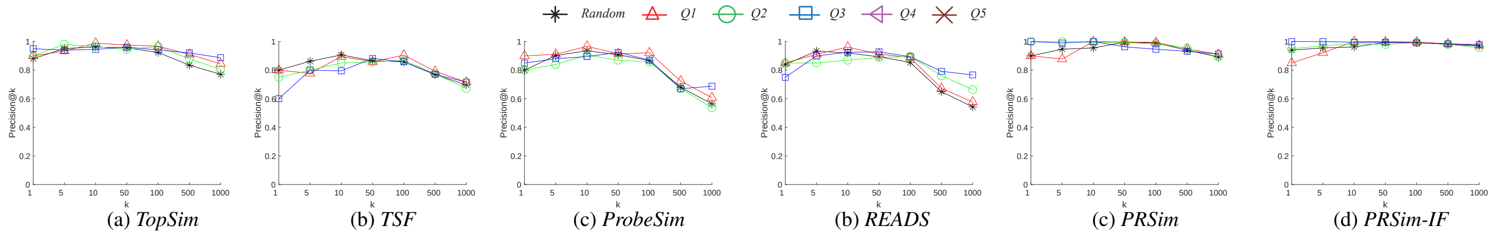


Figure 16: Precision@k on DB, for queries via stratified sampling

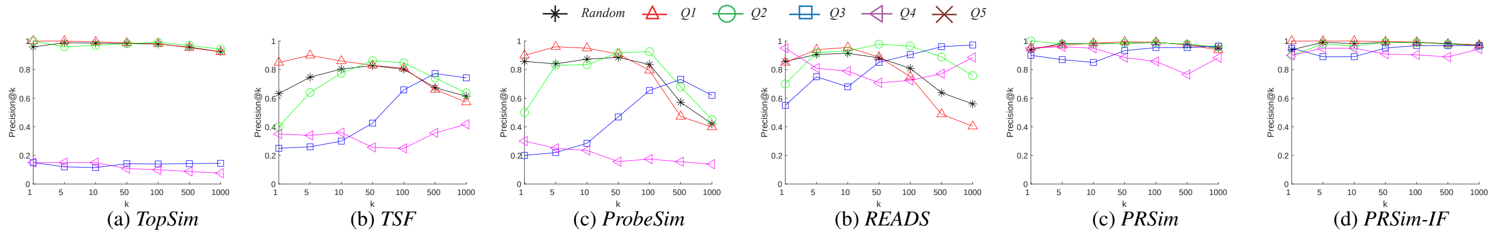


Figure 17: Precision@k on LJ, for queries via stratified sampling

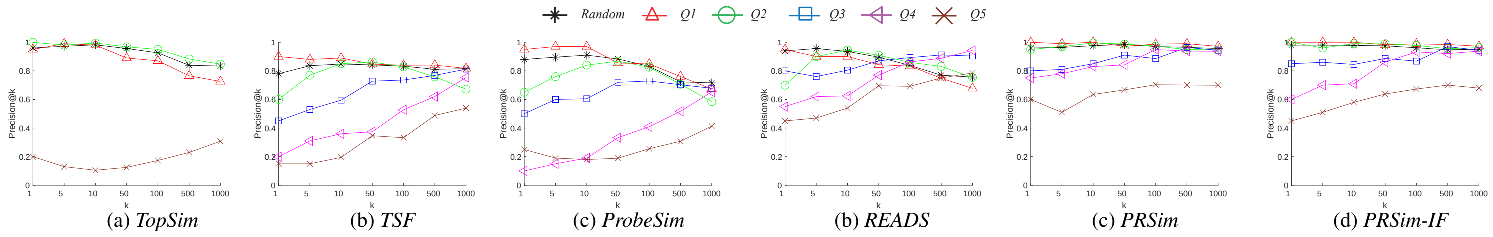
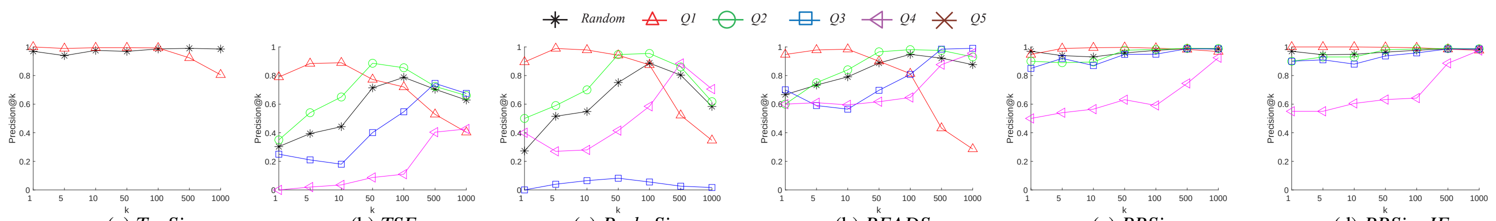
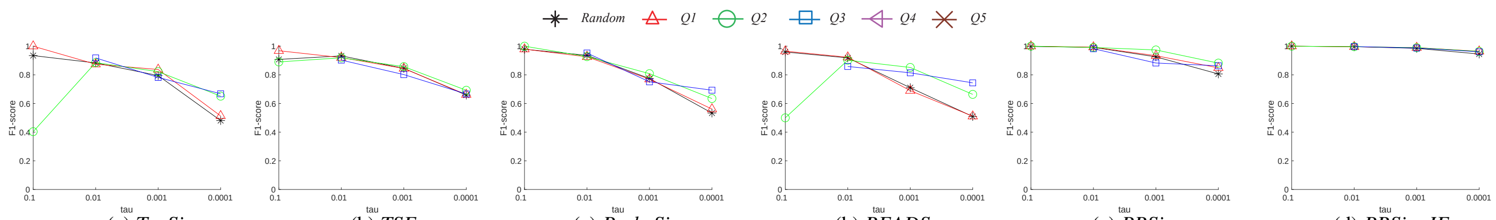


Figure 18: Precision@k on IT, for queries via stratified sampling



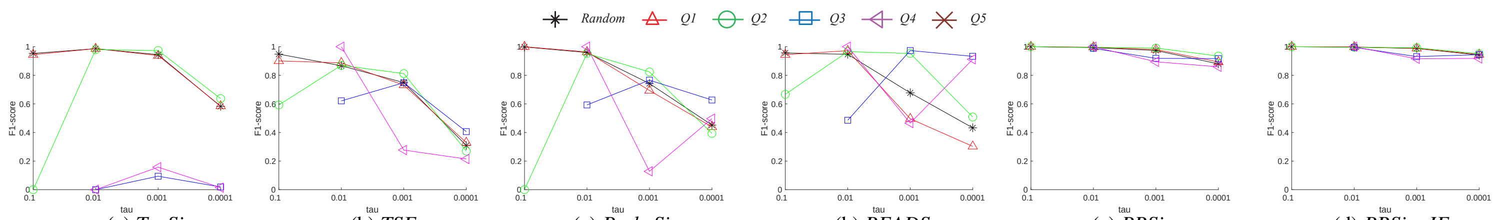
(a) *TopSim* (b) *TSF* (c) *ProbeSim* (b) *READS* (c) *PRSim* (d) *PRSim-IF*

Figure 19: Precision@k on FD, for queries via stratified sampling



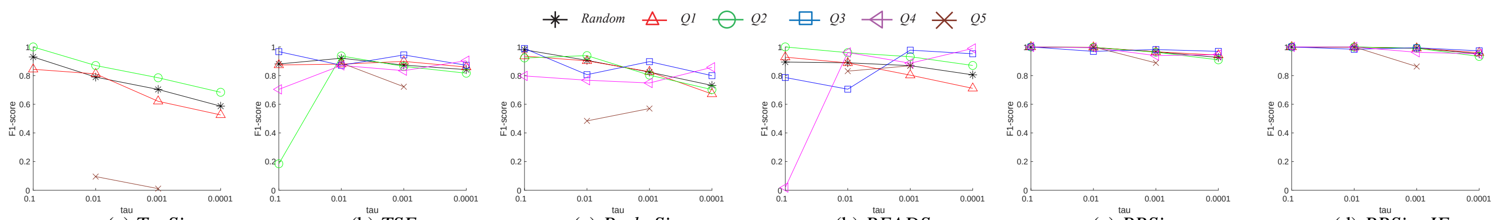
(a) *TopSim* (b) *TSF* (c) *ProbeSim* (b) *READS* (c) *PRSim* (d) *PRSim-IF*

Figure 20: F1-score on DB, for queries via stratified sampling



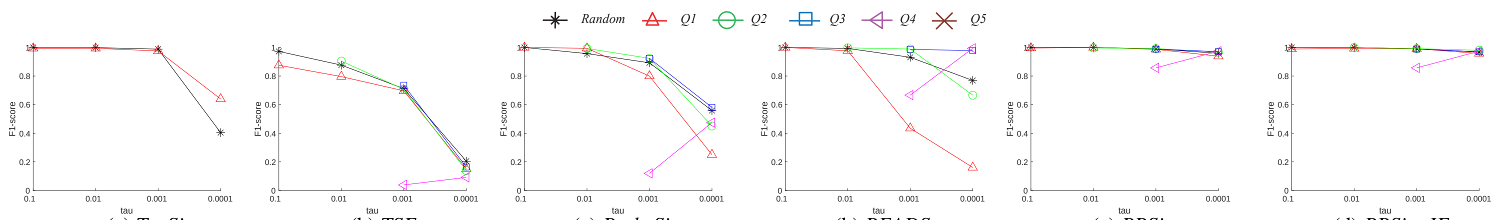
(a) *TopSim* (b) *TSF* (c) *ProbeSim* (b) *READS* (c) *PRSim* (d) *PRSim-IF*

Figure 21: F1-score on LJ, for queries via stratified sampling



(a) *TopSim* (b) *TSF* (c) *ProbeSim* (b) *READS* (c) *PRSim* (d) *PRSim-IF*

Figure 22: F1-score on IT, for queries via stratified sampling



(a) *TopSim* (b) *TSF* (c) *ProbeSim* (b) *READS* (c) *PRSim* (d) *PRSim-IF*

Figure 23: F1-score on FD, for queries via stratified sampling