Approximating All-Pairs Similarity Search by Rademacher Average

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Abstract

All-pairs similarity search (APSS) has abundant applications in many fields such as collaborative filtering, recommendations, search query suggestions, spam detection, etc. This paper proposes two approximation algorithms for cosine similarity based APSS and SimRank based APSS respectively. We have given the upper bounds of the approximation errors for the worst case by using Rademacher average. To the best of our knowledge, we are the first to apply Rademacher average to bound the errors in APSS approximation problems. We also evaluate our algorithms by experiments on real-world data sets to verify that our upper bounds are tight enough for practical use.

1 Introduction

All-pairs similarity search (APSS) has received extensive research interest recently [5, 44, 1, 38]. Collaborative filtering [36], similarity-based recommendations [31], search query suggestions [9], spam and plagiarism detection [11, 27] all find APSS useful in practice. To improve performance, many approximation approaches have been proposed [17, 14, 21, 12]. Hence the computation [5, 13, 44, 1, 38] and approximation [17, 14, 21, 12] of the all-pairs similarities have been popular in research for more than ten years.

This paper considers two approximation methods for cosine similarity based search [37, 44, 1, 38], and SimRank based search [22, 25, 15, 23] respectively. Our solution idea is to treat the cosine similarity or SimRank between two vectors as a true average over random variables, and then we can use sampled average to approximate the true average. We explain the details as follows:

- Cosine similarity between two vectors, each of which contains m features, is defined as

$$Sim(u, v) = \frac{1}{||u|| \cdot ||v||} \sum_{i=1}^{m} u_i \cdot v_i,$$

where $|| \cdot ||$ denotes 2-norm and u_i is the i-th component (feature) value. If we normalize each vector to make their norms all equal to $\sqrt{m}$, then cosine similarity is just the true average of the m feature products between two vectors:

$$Sim(u, v) = \frac{1}{m} \sum_{i=1}^{m} u_i \cdot v_i.$$

Suppose m is large, e.g., over 1K. Then it is time consuming to traverse all the m feature pairs and do the multiplications. A straightforward method to approximate the true average is by using the sampled average

$$\widetilde{Sim}(u, v) = \frac{1}{|S|} \sum_{s_i \in S} u_{s_i} \cdot v_{s_i}.$$

That is, we can choose k out of m features at random, and compute the average of the k sampled feature products as an approximation of the cosine similarity. Thanks to the recent advance in statistical learning theory (especially the results of Rademacher average), there are tight error bounds for this sampling method.

- SimRank between two nodes in the graph can be defined as

$$s(a, b) = \sum_{t:(a,b)(x,x)} P[t] \cdot c^{L(t)},$$

where t is a pair of random walks with the same length $L(t)$, which lead the starting nodes a and b to meet at one node x, and $P[t]$ denotes the probability when t is chosen. Hence SimRank can be treated as the true average of the random variable $c^{L(t)}$, where t is taken over the space of all the pairs of random walks that start from the two nodes respectively. Thus similarly, we can sample over the random walk space and then use the sampled average as an approximation. Again, tight error bounds given by Rademacher average are also inherited.

The approximation error of each our algorithm can be upper bounded by using Rademacher average [4, 29, 3]. We can treat the similarity approximation as a learning problem over large scaled data set. In the analysis, we want to upper bound the approximation error for the worst case, i.e., to bound the maximum error $\overline{E}$ among all pairs:

$$\overline{E} = \max_{u \neq v} |\widetilde{Sim}(u, v) - Sim(u, v)|.$$

Rademacher average does an excellent job on how to bound such maximum error [34, 35]. The key result we use in this paper is that with probability at least $1 - \delta$,

$$\overline{E} \leq R + c \left(1 + \sqrt{\frac{8}{k} \log \frac{2}{\delta}} + \sqrt{\frac{8}{k} \log \frac{2}{\delta} + \frac{8R}{c}} \right) \sqrt{\frac{\log \frac{8}{\delta}}{2k}},$$

where R denotes the Rademacher average of the data set, and k is the number of samples, and c is the number of features for cosine similarity, or the constant between 0 and 1 for SimRank. It is also possible to upper bound the Rademacher average by the state-of-art results [2, 34, 35]. Thus we can find an upper bound of the worst errors for our approximation algorithms.

Our Contributions. We are the first to give the approximation algorithms for APSS that can achieve upper bounds on maximum errors, and to show the upper bounds by using Rademacher average. We also evaluate our algorithms by using real-world data sets.

The rest of this paper is organized as follows. Section 2 discusses the related works. Section 3 introduces the problem settings and reviews some technical background. Section 4 approximates the cosine similarity based APSS and also gives the analysis on the upper bound of maximum errors. Section 5 approximates the SimRank based APSS and also gives an upper bound on maximum errors. 6 evaluates our algorithms and presents the experimental results.

2 Related Works

All-pairs similarity search (APSS) is recently a popular research topic in the community of information retrieval [5, 44, 1, 38]. Given a big set of objects, the goal of APSS is to efficiently compute (or approximate) the similarities between each pair of objects. Many similarity measures have been proposed [37], e.g., Cosine Similarity [39], SimRank [22], Jaccard Index [18], Metric Distance [37], Pearson Correlation [6], etc. For similarity search, Cosine Similarity and SimRank are very popular ([39, 44, 1, 38] for Cosine, and [25, 15, 23, 45] for SimRank). A major challenge of APSS is the large volume of computation: given n objects, without any assumption on the similarity distribution (e.g., the similarity matrix is sparse), the time complexity is at least $O(n^2)$. To compute more efficiently, the state-of-art research works often use parallelism [10, 19] and dissimilarity detection [1, 38]. If only approximations are needed, how to efficiently sample with negligible error for similarity search is another research focus [17, 14, 21, 12]. This paper focuses on the approximation problem.

We may treat the similarity approximation as a learning problem over large scaled data, and we need to upper bound the learning error for the worst case. In statistical learning theory, such upper bounds are usually

called risk bounds [40]. There are two classical methods to compute the risk bounds: by VapnikChervonenkis (VC) dimension [41, 42, 40] and by Rademacher average [29, 4, 3]. Many approximation algorithms that use these two techniques have been proposed [32, 33, 34, 35]. Riondato and Kornaropoulos [32, 33] proposed algorithms that use VC dimension to upper bound the sample size that is sufficient to approximate the betweenness centralities [8] of all nodes in a graph with guaranteed error bounds. One limitation of the VC-based algorithms is that the upper bounds of some characteristic quantities (e.g., the maximum length of any shortest path) are needed [32, 33, 35]. But such bounds are not always available. One year later, Riondato and Upfal used Rademacher average to approximate the frequent itemsets [34] and betweenness centralities [35]. They also found that by using Rademacher average, we can avoid the aforementioned limitation of VC-based solutions. It has been proved that Rademacher average can be applied to various approximation problems, which are out of the scope of classical learning framework. This paper basically follows this idea. To the best of our knowledge, there is no research work connecting similarity approximation with Rademacher average. We attempt to fill this void.

3 Problem Formulation and Preliminaries

3.1 Cosine Similarity

We consider the cosine similarity based all-pairs similarity search. Suppose there are n vectors (each vector can represent a user profile or a web page). Each vector contains m non-negative features. Define the cosine similarity between two vectors u and v as

$$Sim(u, v) = \frac{1}{||u|| \cdot ||v||} \sum_{i=1}^{m} u_i \cdot v_i,$$

where u_i, v_i denotes the i-th feature value of u, v. For simplicity, we assume all the vectors are adjusted with the same norm: $||v|| = \sqrt{m}$ for every v in the n vectors. Then the equation above can be simplified as

$$Sim(u, v) = \frac{1}{m} \sum_{i=1}^{m} u_i \cdot v_i.$$

That is, the similarity is defined as the average on the corresponding feature products between the vectors.

To do the all-pairs similarity search (APSS), we need to compute the similarity between each pair of vectors. Since there are $n(n-1)$ pairs, and for each pair we need m times of multiplication, the total complexity of a naiive algorithm is $O(n^2 m)$. Fortunately, there are many methods to detect dissimilar pairs (two vectors without sharing any feature) [1, 38, 26], which can save a lot of computation. For the state-of-art works, to compute all the pairs, the complexity can be lowered to $O(nkm)$, where k is much less than n. However, to the best of our knowledge, there were few discussions on the size of features m. If we can only consider a part of the m features without significantly deteriorating the accuracy, then the total computation time for APSS can be lowered significantly (note that nk is still large for very big dataset). We can approximating the similarity by sampling on the features.

3.2 SimRank

SimRank [22] is a popular measure of the similarity between two nodes in a graph based on the idea that similar nodes are often referred by other similar nodes. Denote by $s(a, b)$ the SimRank between nodes a and b. If $a = b$, then $s(a, b)$ is defined to be 1. Otherwise,

$$s(a, b) = \frac{c}{|I(a)| \cdot |I(b)|} \sum_{i \in I(a)} \sum_{j \in I(b)} s(i, j),$$

where c is a constant in $(0, 1)$ and $I(a)$ denotes the in-neighbors of a. If there is an edge from a to b, then a is an in-neighbor of b. An important fact is that SimRank can be equivalently built upon Random Surfer-Pairs Model [22]. That is, $s(a, b)$ can also be written as follows:

$$s(a, b) = \sum_{t:(a,b)(x,x)} P[t] \cdot c^{L(t)},$$

where t is a pair of random walks with the same number of steps, which lead a and b to meet at one node x, and $P[t]$ denotes the probability when t is chosen, and $L(t)$ denotes the number of steps of each walk in t. Here we take random walks from the reversed graph, in which each edge is reversed compared with the original graph. A random walk works as follows: in the tour at any node, which has k out-edges, we take one of the k edge with equal probability $1/k$ as our next step. Note that as the length of random walk grows, its contribution to $s(a, b)$ decreases exponentially. Hence in practice, we only need to consider relatively short walks, e.g., with length no more than T.

3.3 Rademacher Average

This section proposes our approximation algorithm and its analysis. Suppose we want to compute the cosine similarities between a fixed vector u and other vectors $v_1, v_2, \cdots, v_n$. We take the m features as the sample space S:

$$S = \{s_1, \cdots, s_k\} \subseteq D$$

where k is the number of samples we take, and D is the feature space: $D = \{1, 2, \cdots, m\}$. Let F be a collection of functions from the features D to the interval $[0, m]$. For each function $f \in F$, define the *true average* $A_D(f)$ and *sampled average* $A_S(f)$ as follows:

$$A_D(f) = \frac{1}{m} \sum_{i=1}^{m} f(i), \quad A_S(f) = \frac{1}{k} \sum_{i=1}^{k} f(s_i).$$

Define the *uniform deviation* [30] of F given S as

$$U_S(F) = \sup_{f \in F} [A_S(f) - A_D(f)].$$

Note that if F is a finite set (in this paper we will see this is true), supreme can be replaced by maximum:

$$U_S(F) = \max_{f \in F} [A_S(f) - A_D(f)].$$

Define the *Rademacher average* [29, 4, 30] of F given S as

$$R_S(F) = \mathbb{E}_\sigma \left[\sup_{f \in F} \frac{2}{k} \sum_{i=1}^{k} \sigma_i f(s_i) \right],$$

where each σ_i is a random variable uniformly distributed over $\{-1, 1\}$, and the mean $\mathbb{E}_\sigma$ takes randomness over all the σ_i's conditionally on S. Again, one can replace supreme by maximum.

The main motivation of our algorithm is that the difference between true average and sampled average is upper bounded by the Rademacher average as follows. We leave the proofs to the Appendix.

Theorem 1. Let F be a collection of functions f mapping D to $[0, m]$. With probability at least $1 - \delta$, we have

$$\sup_{f \in F} |A_S(f) - A_D(f)| \leq R_S(F) + \left(m + m\sqrt{\frac{8}{k} \log \frac{2}{\delta}} + m\sqrt{\frac{8}{k} \log \frac{2}{\delta} + \frac{8R_S(F)}{m}} \right) \sqrt{\frac{\log \frac{8}{\delta}}{2k}}.$$

The remaining item we need to upper bound is $R_S(F)$. Our result is similar to Massart's lemma [2].

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Theorem 2.
$$R_S(F) \leq \frac{\ell}{k} \sqrt{8 \log |F|},$$

where $\ell^2 = \sup_{f \in F} \sum_{i=1}^{k} f(s_i)^2$.

By the above two theorems, we can bound our approximation error even for the worst case.

4   Approximating Cosine Similarities

The approximation algorithm takes as input a collection of n vectors V and two parameters (ϵ, δ) whose values are between 0 and 1. The algorithm outputs a set $C = \{\tilde{S}(u,v) : u, v \in V, u \neq v\}$, where $\tilde{S}(u,v)$ is the (ϵ, δ)- approximation of cosine similarity between u and v, i.e., with probability at least $1 - \delta$, the worst approximation error in C is at most ϵ. Each vector in V contains m features. We take the m features as the sample space $D = \{1, \cdots, m\}$. For each feature $s \in D$, let $f_{u,v}(s) = u_s \cdot v_s$, where u_s is the s-th feature value of the vector u. Let $F = \{f_{u,v} : u, v \in V, u \neq v\}$. Thus $|F| < n^2/2$ since symmetry of cosine similarity. It is clear that the true average of $f_{u,v}$ equals to the cosine similarity between u and v. Given the sampled features, the upper bound of $R_S(F)$ is

$$R_S(F) \leq \frac{\ell}{k} \sqrt{8 \log |F|} < \frac{4\ell \sqrt{\log n}}{k},$$

where $\ell = \sqrt{\max_{f \in F} \sum_{i=1}^{k} f(s_i)^2}$. Since F is finite, we can replace supreme by maximum.

4.1   The Algorithm

The approximation algorithm works in an iterative mode. For each iteration, we sample some new features s_i's among D and aggregate the feature products given by $f_{u,v}(s_i)$ for each $f_{u,v}$ in F. Then we compute the error upper bound:

$$\Delta = \frac{4\ell \sqrt{\log n}}{k} + \left(m + m\sqrt{\frac{8}{k} \log \frac{2}{\delta}} + m\sqrt{\frac{8}{k} \log \frac{2}{\delta}} + \frac{32\ell \sqrt{\log n}}{mk} \right) \sqrt{\frac{\log \frac{8}{\delta}}{2k}},$$

where $\ell = \sqrt{\max_{f \in F} \sum_{i=1}^{k} f(s_i)^2}$, and k is the number of aggregated samples. If $\Delta \leq \epsilon$, then we stop and return the averages $\frac{1}{k} \sum_{s_i \in S} f_{u,v}(s_i)$ for each pair u, v. Otherwise, we continue to the next round, where we will sample more features. If $\Delta \leq \epsilon$ can never be satisfied, at the end we will sample all the m features and return the averages as the exact solution. Algorithm 1 gives the pseudocode of our solution.

It is clear to verify the correctness of our algorithm by Theorem 1 and Theorem 2.

4.2   Improving the Upper Bound

Note that in the upper bound Δ of Algorithm 1, m is a dominating variable: it is proportional to Δ. Usually m can be quite large, e.g., from 100 to 10K. Thus it is worth investigating how to mitigate the negative effect of large m. The idea comes from Theorem 1, which assumes the range of each function f is $[0, m]$. However in reality, most feature products $u[s] \cdot v[s]$ are close to zero due to sparsity, and its maximum value shall be much less than m. In practice, usually we can assume there is a good estimation (much less than m) on the maximum feature product based on historic experience. To further lower the upper bound Δ, a variant of Algorithm 1 may use the bound as follows:

$$\hat{m} = \max_{i \in [1, \cdots, m], u, v \in V, u \neq v} u[i] \cdot v[i],$$

Algorithm 1 Cosine Similarity Approximation

Input: vectors V ($|V| = n$); features U ($|U| = m$); $\epsilon \in (0,1)$; $\delta \in (0,1)$.
Output: $Sim(u,v)$ for each $u,v \in V$ s.t. $u \neq v$.
  $k \leftarrow 0$;
  $S \leftarrow \emptyset$;
  $S(u,v) \leftarrow 0$ for each $u,v \in V$ s.t. $u \neq v$;
  while $k \leq m$ **do**
    $k' \leftarrow \mathsf{next-sample-size}(k)$;
    for i from k to $k'-1$ **do**
      Uniformly sample a feature s from $U \setminus S$;
      $S(u,v) \leftarrow S(u,v) + u[s] \cdot v[s]$;
      $S \leftarrow S \cup \{s\}$;
    end for
    $\Delta \leftarrow \frac{4\ell\sqrt{\log n}}{k} + \left(m + m\sqrt{\frac{8}{k}\log\frac{2}{\delta}} + m\sqrt{\frac{8}{k}\log\frac{2}{\delta} + \frac{32\ell\sqrt{\log n}}{mk}} \right)\sqrt{\frac{\log\frac{8}{\delta}}{2k}}$;
    if $\Delta \leq \epsilon$ **then**
      break the while loop;
    end if
  end while
  $\mathsf{S} \leftarrow \{S(u,v)/k : u,v \in V, u \neq v\}$.
  return S.

---

where $[1, \cdots, m]$ denotes all the m features, and V is the set of all vectors. Intuitively, $\hat{m}$ is the maximum value of all the feature products, and we assume we have a good estimation of $\hat{m}$. Then we may choose the upper bound as follows:

$$\Delta = \frac{4\ell\sqrt{\log n}}{k} + \hat{m}\left(1 + \sqrt{\frac{8}{k}\log\frac{2}{\delta}} + \sqrt{\frac{8}{k}\log\frac{2}{\delta} + \frac{32\ell\sqrt{\log n}}{\hat{m}k}} \right)\sqrt{\frac{\log\frac{8}{\delta}}{2k}}.$$

We use experiments (in Section 6) to show that the improvement of the variant above is significant.

5   Approximating SimRank

We approximate SimRank scores on the nodes in the digraph $G = (V, E)$. The basic idea is similar to the case of cosine similarity approximation, but the sample space D is changed to the $2T$-dimensional manifold $[0,1]^{2T}$, where $[0,1]$ is the interval of real numbers between 0 and 1, and F is now defined as

$$F = \{f_{a,b} : a,b \in V, a \neq b\},$$

where given any two nodes a, b, the function $f_{a,b}$ takes a sample $s_i \in D$ as input and outputs a value in the interval $[0, c]$. Algorithm 2 shows how to generate a random walk given a sample from $[0,1]^T$ and a starting node a. It is clear that the random walk chosen by Algorithm 2 is uniformly distributed if the sample is uniformly drawn from $[0,1]^T$. Thus given two nodes a, b and a sample $s_i \in [0,1]^{2T}$, we can generate two random walks W_a, W_b starting from a and b respectively. Let

$$l_{a,b}(s_i) = \min\{j : 1 \leq j \leq T, W_a[j] = W_b[j]\},$$

i.e., the number of steps before two surfers starting from a, b meet at some node. If W_a and W_b never meet within T steps, $l_{a,b}(s_i)$ is defined to be 0.

The function $f_{a,b}(s_i)$ is defined as

$$f_{a,b}(s_i) = \begin{cases} 0 & \text{if } l_{a,b}(s_i) = 0, \\ c^{l_{a,b}(s_i)} & \text{otherwise.} \end{cases}$$

Algorithm 2 Random Walk Generation
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Input: reversed graph $\overline{G}$, sequence $(s_1, \cdots, s_T) \in [0, 1]^T$, starting node a.
Output: a random walk $W = (a, \cdots)$ starting from a.
  Let W be a sequence of length $T + 1$;
  $W[0] \leftarrow a$;
  for i from 1 to T **do**
    $I \leftarrow \{b : \text{there is an edge in } \overline{G} \text{ from } W[i-1] \text{ to } b\}$;
    $k \leftarrow |I|$;
    if k=0 **then**
      $W[i] \leftarrow W[i-1]$;
    else
      Sort I in lexicographical order: $(I[0], \cdots, I[k-1])$;
      $x \leftarrow \lfloor s_{i-1} * k \rfloor$;
      $W[i] \leftarrow I[x]$;
    end if
  end for
  return W.
___

It is clear that the true average $A_D(f_{a,b})$ equals to the SimRank between the nodes a and b. Thus a similar approximation idea based on Rademacher average can be applied. We still need to upper bound the worst approximation error. The new bound is stated as follows.

Theorem 3. Let F be a collection of functions f mapping D to $[0, c]$. With probability at least $1 - \delta$, we have

$$\sup_{f \in F} |A_S(f) - A_D(f)| \leq R_S(F) + \left(c + c\sqrt{\frac{8}{k} \log \frac{2}{\delta}} + c\sqrt{\frac{8}{k} \log \frac{2}{\delta} + \frac{8R_S(F)}{c}} \right) \sqrt{\frac{\log \frac{8}{\delta}}{2k}}.$$

The proof is essentially the same as the proof of Theorem 1. We leave the discussions to the Appendix. Also the upper bound of $R_S(F)$ given by Theorem 2 remains unchanged.

Our approximation algorithm works as follows. For each iteration, we sample some new features s_i's among D, generate random walks W_a, W_b from nodes a, b given s_i and aggregate $f_{a,b}(s_i)$ for each $f_{a,b}$ in F. Then we compute the error upper bound:

$$\Delta = \frac{4\ell\sqrt{\log n}}{k} + \left(c + c\sqrt{\frac{8}{k} \log \frac{2}{\delta}} + c\sqrt{\frac{8}{k} \log \frac{2}{\delta} + \frac{32\ell\sqrt{\log n}}{ck}} \right) \sqrt{\frac{\log \frac{8}{\delta}}{2k}},$$

where $\ell = \sqrt{\max_{f \in F} \sum_{i=1}^{k} f(s_i)^2}$, and k is the aggregated samples. If $\Delta \leq \epsilon$, then we stop and return the averages $\frac{1}{k} \sum_{s_i \in S} f_{a,b}(s_i)$ for each pair u, v. Otherwise, we continue to the next round, where we will sample more features. If $\Delta \leq \epsilon$ can never be satisfied with a certain number of iterations, we return the approximated SimRank scores of node pairs, with the message that the input parameters (ϵ, δ) cannot be satisfied by our algorithm.

It is clear to verify the correctness of our algorithm by Theorem 3 and Theorem 2.

6 Evaluation

In this section we evaluate our algorithms. We use both synthesized and real-world data sets.

Algorithm 3 SimRank Approximation

Input: reversed graph $\overline{G}$; $\epsilon \in (0,1)$; $\delta \in (0,1)$; maximum random walk length T; maximum number of iterations R; SimRank constant c.
Output: SimRank(u,v) for each $u,v \in V$ s.t. $u \neq v$.
   $k \leftarrow 0$;
   $S(u,v) \leftarrow 0$ for each $u,v \in V$ s.t. $u \neq v$;
   for count from 1 to R **do**
      $k' \leftarrow \mathsf{next - sample - size}(k)$;
      for i from k to $k'-1$ **do**
         Uniformly sample a feature s from $[0,1]^{2T}$;
         for each $a,b \in V \times V$ s.t. $a \neq b$ **do**
            $W_a \leftarrow$ Random Walk Generation$(s[1 \cdots T])$;
            $W_b \leftarrow$ Random Walk Generation$(s[(T+1)\cdots 2T])$;
            $L \leftarrow \{j : 1 \leq j \leq T, W_a[j] = W_b[j]\}$;
            if $|L| > 0$ **then**
               $l_{a,b} \leftarrow \min L$;
               $S(u,v) \leftarrow S(u,v) + c^{l_{a,b}}$;
            end if
         end for
      end for
      $\Delta \leftarrow \frac{4\ell\sqrt{\log n}}{k} + \left(c + c\sqrt{\frac{8}{k}\log\frac{2}{\delta}} + c\sqrt{\frac{8}{k}\log\frac{2}{\delta} + \frac{32\ell\sqrt{\log n}}{ck}}\right)\sqrt{\frac{\log\frac{8}{\delta}}{2k}}$;
      if $\Delta \leq \epsilon$ **then**
         break the while loop;
      end if
   end for
   $\mathsf{S} \leftarrow \{S(u,v)/k : u,v \in V, u \neq v\}$.
   if count $= R$ **then**
      show a message that (ϵ, δ) cannot be satisfied.
   end if
   return S.

6.1 Setup

We implemented our algorithms by Python 3.4.3 and ran the programs on a Fedora 20 (Linux) cluster. Every measurement was averaged over 100 test cases, i.e., we ran our algorithms on 100 random vector collections or 100 random graphs and then computed the average.

- **Synthesized data sets**

  For the cosine similarity approximation, we have 100 vectors with 1000 features. We considered two distributions of the feature values: uniform distribution and normal distribution. For uniform distribution, each feature value uniformly distributes over the interval $[0,1]$. For normal distribution, each feature value is generated by $|X|$, where X is a random variable of standard normal distribution $\mathcal{N}(0,1)$. At last, each vector was normalized with norm $\sqrt{m}$. We set the error probability $\delta = 0.0001$.

  For the SimRank approximation, we have 100 nodes in total. We implemented two graph models: random graph model [16] and small-world model [43]. In random graph model, each pair of nodes are connected by an edge with probability $p = 0.1$. In small-world model, each node is connected by an edge with its 4 nearest neighbors, and each other pair of nodes are connected by an edge with probability $p = 0.1$. We choose the constant $c = 0.7$. We set the error probability $\delta = 0.0001$.
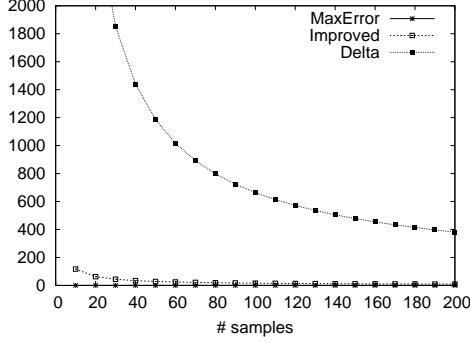
- **Real-world data sets**

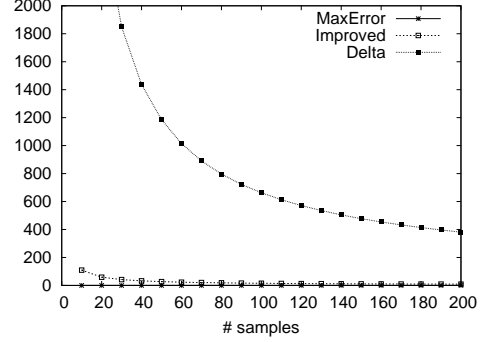Figure 1: MaxErrors and upper bounds for cosine similarity with normal distribution.

Figure 2: MaxError and upper bounds for cosine similarity with uniform distribution.

For the cosine similarity approximation, we use `Cit-HepPh` and `Email-Enron` from Stanford Large Network Dataset Collection (SNAP) [24]. `Cit-HepPh` has 34551 vectors, each of which has 34551 features. `Email-Enron` has 36697 vectors, each of which has 36697 features.

For the SimRank approximation, we use two networks from `ego-Twitter` and `ego-Gplus` from SNAP. The network from `ego-Twitter` has 95 nodes and 951 edges. The network from `ego-Gplus` has 344 nodes and 4178 edges.

6.2 Approximation Errors and Sample Sizes

Figure 1 and Figure 2 present the maximum approximation errors and upper bound given by Algorithm 1 for the synthesized data sets. Here MaxError denotes the maximum absolute error among all the vector pairs, i.e.,

$$\text{MaxError} = \max_{u,v \in V, u \neq v} |\widetilde{Sim}(u,v) - Sim(u,v)|,$$

where $\widetilde{Sim}(u,v)$ is the approximated similarity between u and v given by our algorithms. The upper bound Delta is the Δ given in Algorithm 1, and the improved bound is given in Section 4.2. For the improved bound, we observe that with overwhelming probability, each feature product between any two vectors is less than 20.0 when $m = 1000$. Hence we choose the adjusted parameter $\hat{m} = 20.0$. See Section 4.2 for details. For both figures, when more samples are drawn, the maximum absolute errors and upper bounds decrease. Also our improved upper bounds are significantly tighter than the bounds by m, but they are still much larger than the maximum absolute errors. Hence our theoretical bounds are still quite loose. However, our improved bounds can be sufficient for practical use. For uniform distribution, by 200 samplings, we can guarantee that the maximum absolute error among all the vector pairs is less than 9.0 with probability at least 99.99%. Note that the cosine similarities can be between 0 and $m = 1000$. Thus 9.0 is relatively small. Similarly for normal distribution, by 190 samplings we can guarantee that with probability at least 99.99%, the maximum absolute error is less than 10.0.

Figure 3 and Figure 4 give the maximum approximation errors and upper bound given by Algorithm 1 for the real-world data sets. Since there are more features (more than 30K), the upper bounds cannot be as tight as before. However, for `Cit-HepPh`, only 200 samples can guarantee an upper bound 27.2, which is quite small compared to the number of features.

Figure 5 and Figure 6 present the approximation errors and upper bound given by Algorithm 3 for the synthesized data sets. Here the upper bound Delta is given in Algorithm 3. MaxError is same as before. For both figures, when more samples are drawn, the maximum absolute errors and upper bounds decrease. Note that even though our bounds are still quite loose compared to the maximum absolute errors, they can be practically used. For random graph model, by taking 10000 samples, we can guarantee that the maximum
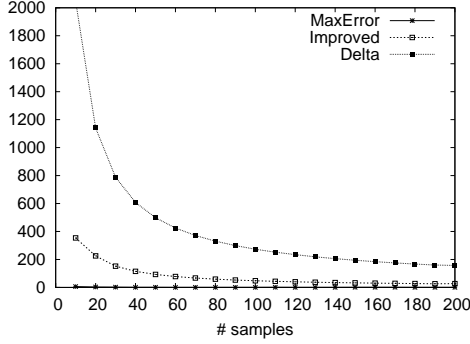
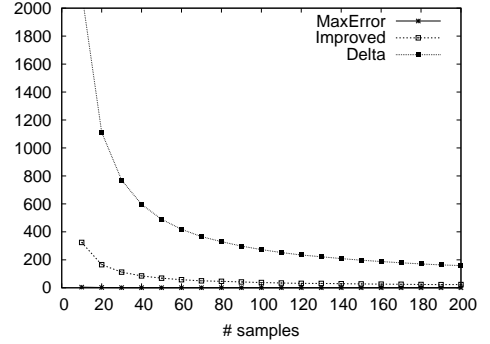Figure 3: MaxErrors and upper bounds for cosine similarity for `Cit-HepPh`.

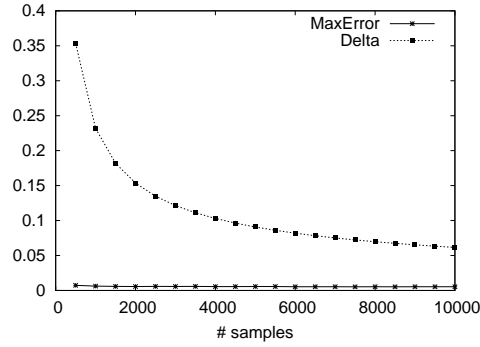Figure 4: MaxError and upper bounds for cosine similarity for `Email-Enron`.

Figure 5: MaxError and upper bounds for Sim-Rank with random graph model.
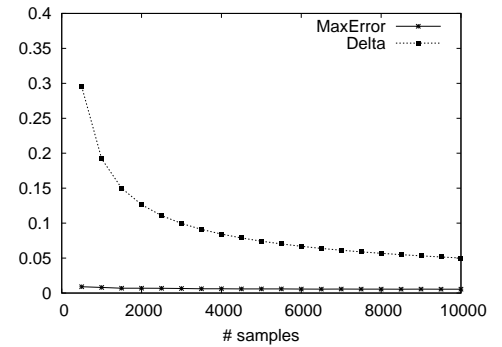

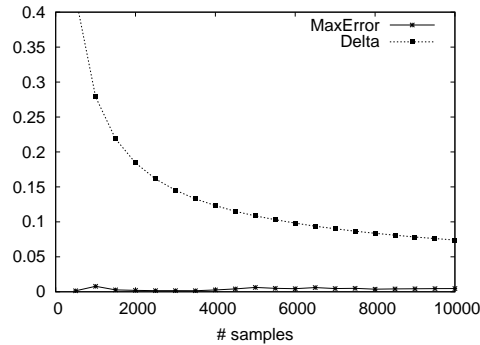Figure 6: MaxError and upper bounds for Sim-Rank with small-world model.

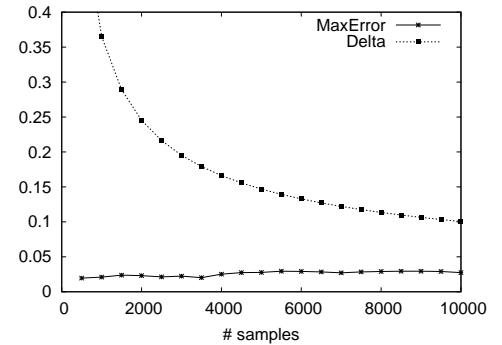Figure 7: MaxError and upper bounds for Sim-Rank for the network from `ego-Twitter`.

Figure 8: MaxError and upper bounds for Sim-Rank for the network from `ego-Gplus`.

absolute error among all the node pairs is less than 0.062 with probability at least 99.99%. For small-world model, by taking 10000 samples, we can guarantee that the maximum absolute error is less than 0.051 with probability at least 99.99%.

Figure 7 and Figure 8 give the maximum approximation errors and upper bound given by Algorithm 3 for the real-world data sets. The upper bounds are not as tight as before. For `ego-Twitter`, 10000 samples
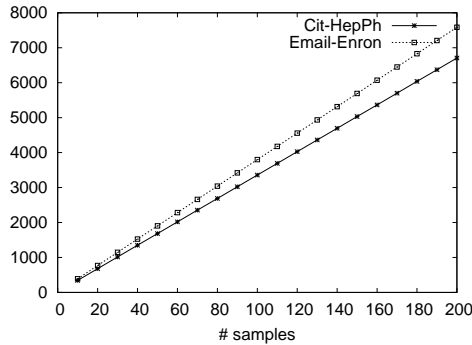
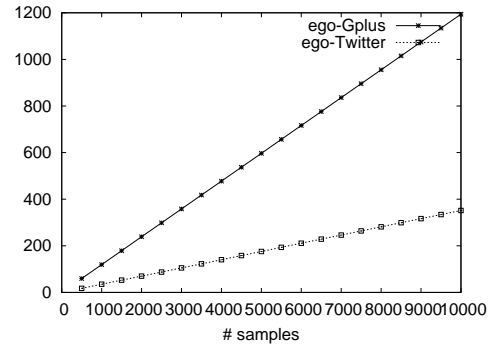Figure 9: Running time of Algorithm 1 given sample sizes.

Figure 10: Running time of Algorithm 3 given sample sizes.

can guarantee an upper bound of 0.074. For `ego-Gplus`, 10000 samples can guarantee an upper bound of 0.10.

6.3 Running Time

Figure 9 and Figure 10 give the running time of our algorithms on the real-world data sets given the sample sizes. Here we did not use any parallelism or detection techniques to implement our algorithms. Note that in APSS we need to compute for each pair of objects. The number of such pairs grows quadratically. As a result when the sample size is large, the computation can take a few hours. A good news is that since the computation of each pair is independent from each other, the approximation algorithms can be easily distributed over multiple cores.

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7 Appendix

7.1 Proof of Theorem 1

In this section, we show our main result (Theorem 1). We start from the definition of self bounding function [30].

Definition 1. *Let s_1, s_2, $\cdots$, s_k be independent random variables taking values from a set D. A function $f : D^k \to [0, +\infty]$ is a self bounding function if there exists a constant c and a function $g : D^{k-1} \to \mathbb{R}$ such that for any $s_1, \cdots, s_{j-1}, s_{j+1}, \cdots, s_k \in D$, the following conditions hold:*

$$0 \le f(s_1, \cdots, s_k) - g(s_1, \cdots, s_{j-1}, s_{j+1}, \cdots, s_k) \le c,$$

$$\sum_{j=1}^{k} [f(s_1, \cdots, s_k) - g(s_1, \cdots, s_{j-1}, s_{j+1}, \cdots, s_k)] \le f(s_1, \cdots, s_k).$$

The following concentration inequality can be achieved for self bounding functions [7].

Lemma 1. *[7] If a function $Z = f(s_1, \cdots, s_k)$ is a self bounding function with constant c, then for $t \le \mathbb{E}Z$,*

$$\Pr[\mathbb{E}Z - Z \ge t] \le \exp\left(-\frac{t^2}{2c\mathbb{E}Z}\right).$$

For $t > \mathbb{E}Z$, the left probability is zero trivially. Here we take randomness over s_1, s_2, $\cdots$, s_k.

By using the above lemma, we can show a similar inequality for Rademacher average.

Lemma 2.
$$\Pr[\mathbb{E}R_S(F) \ge R_S(F) + t] \le \exp\left(-\frac{kt^2}{4m\mathbb{E}R_S(F)}\right),$$

where $\mathbb{E}$ takes randomness over the samplings s_1, s_2, $\cdots$, s_k.

Proof. It suffices to show that $R_S(F)$ is a self bounding function with constant $c = 2m/k$. Define

$$Z = R_S(F) = \mathbb{E}_\sigma \sup_{f \in F} \left[\frac{2}{k} \sum_{i=1}^{k} \sigma_i f(s_i) \right],$$

$$G_j = \mathbb{E}_\sigma \sup_{f \in F} \left[\frac{2}{k} \sum_{i \neq j} \sigma_i f(s_i) \right].$$

It is clear that Z is non-negative:

$$Z \geq \sup_{f \in F} \left[\mathbb{E}_\sigma \frac{2}{k} \sum_{i=1}^{k} \sigma_i f(s_i) \right] = 0.$$

Also it is clear that $Z \geq G_j$ for each j: suppose $\tilde{f}$ achieves the supreme of G_j. Then

$$G_j = \mathbb{E}_\sigma \left[\frac{2}{k} \sum_{i=1}^{k} \sigma_i \tilde{f}(s_i) - \frac{2}{k} \sigma_j \tilde{f}(s_j) \right]$$

$$= \mathbb{E}_\sigma \left[\frac{2}{k} \sum_{i=1}^{k} \sigma_i \tilde{f}(s_i) \right] - \mathbb{E}_\sigma \left[\frac{2}{k} \sigma_j \tilde{f}(s_j) \right]$$

$$= \mathbb{E}_\sigma \left[\frac{2}{k} \sum_{i=1}^{k} \sigma_i \tilde{f}(s_i) \right] \leq Z.$$

Next we show $Z - G_j \leq 2m/k = c$:

$$G_j = \mathbb{E}_\sigma \sup_{f \in F} \left[\frac{2}{k} \sum_{i=1}^{k} \sigma_i f(s_i) - \frac{2}{k} \sigma_j f(s_j) \right]$$

$$\geq \mathbb{E}_\sigma \sup_{f \in F} \left[\frac{2}{k} \sum_{i=1}^{k} \sigma_i f(s_i) \right] - \mathbb{E}_\sigma \sup_{f \in F} \left[\frac{2}{k} \sigma_j f(s_j) \right]$$

$$\geq \mathbb{E}_\sigma \sup_{f \in F} \left[\frac{2}{k} \sum_{i=1}^{k} \sigma_i f(s_i) \right] - \frac{2m}{k}.$$

Finally we need to verify $\sum_{j=1}^{k} Z - G_j \leq Z$:

$$\sum_{j=1}^{k} G_j = \mathbb{E}_\sigma \sum_{j=1}^{k} \sup_{f \in F} \left[\frac{2}{k} \sum_{i \neq j} \sigma_i f(s_i) \right]$$

$$\geq \mathbb{E}_\sigma \sup_{f \in F} \left[\frac{2}{k} \sum_{j=1}^{k} \sum_{i \neq j} \sigma_i f(s_i) \right]$$

$$= \frac{2(k-1)}{k} \mathbb{E}_\sigma \sup_{f \in F} \left[\sum_{j=1}^{k} \sigma_i f(s_i) \right] = (k-1)Z.$$

$\square$

We still need the following lemma on the relation between uniform deviation and Rademacher average.

Lemma 3.

$$\mathbb{E}\sup_{f\in F}[A_S(f) - A_D(f)] \leq \mathbb{E}R_S(F),$$

$$\mathbb{E}\sup_{f\in F}[A_D(f) - A_F(f)] \leq \mathbb{E}R_S(F).$$

Here we take randomness over the k samplings.

Proof. The proof idea is based on ghost samplings, i.e., independently draw another k samples: $s'_1, \cdots, s'_k$, and then we have

$$A_D(f) = \frac{1}{m}\sum_{i=1}^{m} f(i) = \mathbb{E}\frac{1}{k}\sum_{j=1}^{k} f(s'_j),$$

where $\mathbb{E}$ takes randomness over the k ghost samples. Thus

$$\mathbb{E}\sup_{f\in F}[A_S(f) - A_D(f)] = \mathbb{E}\sup_{f\in F}\left[\frac{1}{k}\sum_{i=1}^{k} f(s_i) - \mathbb{E}\frac{1}{k}\sum_{j=1}^{k} f(s'_j)\right]$$

$$\leq \mathbb{E}\sup_{f\in F}\left[\frac{1}{k}\sum_{i=1}^{k} f(s_i) - \frac{1}{k}\sum_{j=1}^{k} f(s'_j)\right].$$

Since all the samples s, s' are independently identically distributed, flipping the sign of $f(s_i) - f(s'_i)$ will not change the expected supreme, i.e.,

$$\mathbb{E}\sup_{f\in F}\left[\frac{1}{k}\sum_{i=1}^{k} f(s_i) - \frac{1}{k}\sum_{j=1}^{k} f(s'_j)\right] = \mathbb{E}\sup_{f\in F}\frac{1}{k}\sum_{i=1}^{k}[\sigma_i(f(s_i) - f(s'_i))],$$

where σ_i is uniformly distributed over $\{-1, 1\}$. Since

$$\mathbb{E}\sup_{f\in F}\frac{1}{k}\sum_{i=1}^{k}[\sigma_i(f(s_i) - f(s'_i))] \leq 2\mathbb{E}\sup_{f\in F}\frac{1}{k}\sum_{i=1}^{k}\sigma_i f(s_i) = \mathbb{E}R_S(F),$$

we have shown the first inequality. The second inequality is analogous. $\qquad\square$

We also need McDiarmid's inequality [28].

Lemma 4. *[28] Let $s_1, \cdots, s_k$ be independent random variables taking values from a set D. Suppose a function $h : D^k \to \mathbb{R}$ satisfies*

$$\sup_{x_1,\cdots,x_k,x'_i \in D} |h(x_1, \cdots, x_k) - h(x_1, \cdots, x_{i-1}, x'_i, x_{i+1}, \cdots, x_k)| \leq c_i$$

for some constants c_i and every $1 \leq i \leq k$. Then for any $t > 0$, we have

$$\Pr[h(s_1, \cdots, s_k) - \mathbb{E}h(s_1, \cdots, s_k) \geq t] \leq \exp\left(-\frac{2t^2}{\sum_{i=1}^{k} c_i^2}\right).$$

By the above three lemmas, we can bound the difference between true average and sampled average as follows.

Lemma 5.

$$\Pr\left[\sup_{f\in F}|A_D(f) - A_S(f)| \geq R_S(F) + t\right]$$

$$\leq 4\exp\left(-\frac{2kt^2}{(m + \sqrt{8m\mathbb{E}R_S(F)})^2}\right).$$

Proof. First by Lemma 3,

$$\Pr\left[\sup_{f\in F}[A_D(f) - A_S(f)] \geq R_S(F) + t\right]$$

$$\leq \Pr\left[\sup_{f\in F}[A_D(f) - A_S(f)] \geq \mathbb{E}\sup_{f\in F}[A_D(f) - A_S(f)] + at\right]$$

$$+ \Pr\left[\mathbb{E}R_S(F) \geq R_S(F) + (1-a)t\right]$$

for any $a \in [0,1]$. Let

$$h(s_1, \cdots, s_k) = A_D(f) - A_S(f) = A_D(f) - \frac{1}{k}\sum_{i=1}^{k} f(s_i).$$

It is clear that

$$\sup_{x_1,\cdots,x_k,x_i'\in D} |h(x_1, \cdots, x_k) - h(x_1, \cdots, x_{i-1}, x_i', x_{i+1}, \cdots, x_k)|$$

$$= \sup_{x_1,\cdots,x_k,x_i'\in D} \left|\frac{1}{k}\sum_{j=1,j\neq i}^{k} f(x_j) + \frac{1}{k}f(x_i') - \frac{1}{k}\sum_{i=1}^{k} f(x_i)\right|$$

$$= \sup_{x_1,\cdots,x_k,x_i'\in D} \left|\frac{1}{k}f(x_i') - \frac{1}{k}f(x_i)\right| \leq \frac{m}{k}.$$

By McDiarmid's inequality,

$$\Pr\left[\sup_{f\in F}[A_D(f) - A_S(f)] \geq \mathbb{E}\sup_{f\in F}[A_D(f) - A_S(f)] + at\right]$$

$$\leq \exp\left(-\frac{2a^2t^2}{\sum_{i=1}^{k} m^2/k^2}\right) = \exp\left(-\frac{2ka^2t^2}{m^2}\right).$$

By Lemma 2,

$$\Pr\left[\mathbb{E}R_S(F) \geq R_S(F) + (1-a)t\right] \leq \exp\left(-\frac{k(1-a)^2t^2}{4m\mathbb{E}R_S(F)}\right).$$

Let $a = 1/(1 + \sqrt{8\mathbb{E}R_S(F)/m})$. Then putting everything together, we have

$$\Pr\left[\sup_{f\in F}[A_D(f) - A_S(f)] \geq R_S(F) + t\right]$$

$$\leq 2\exp\left(-\frac{2kt^2}{(m + \sqrt{8m\mathbb{E}R_S(F)})^2}\right).$$

Similarly one can show

$$\Pr\left[\sup_{f\in F}[A_S(f) - A_D(f)] \geq R_S(F) + t\right]$$

$$\leq 2\exp\left(-\frac{2kt^2}{(m + \sqrt{8m\mathbb{E}R_S(F)})^2}\right).$$

Thus we have the inequality as desired. □

By the above lemma we have the following important corollary.

Corollary 1. *With probability at least $1 - \delta$, we have*

$$\sup_{f \in F} |A_S(f) - A_D(f)| \leq R_S(F) + (m + \sqrt{8m \mathbb{E} R_S(F)}) \sqrt{\frac{\log \frac{4}{\delta}}{2k}}.$$

We still need to upper bound $\mathbb{E} R_S(F)$. By Lemma 2, with probability at least $1 - \delta$,

$$\mathbb{E} R_S(F) \leq R_S(F) + \sqrt{4m \mathbb{E} R_S(F) \frac{\log \frac{1}{\delta}}{k}}.$$

Or equivalently,

$$\sqrt{\mathbb{E} R_S(F)} \leq \sqrt{\frac{m}{k} \log \frac{1}{\delta}} + \sqrt{\frac{m}{k} \log \frac{1}{\delta} + R_S(F)}.$$

Hence with probability at least $1 - 2\delta$, we have

$$\sup_{f \in F} |A_S(f) - A_D(f)| \leq R_S(F) + \left(m + m\sqrt{\frac{8}{k} \log \frac{1}{\delta}} + m\sqrt{\frac{8}{k} \log \frac{1}{\delta} + \frac{8R_S(F)}{m}} \right) \sqrt{\frac{\log \frac{4}{\delta}}{2k}}.$$

We have shown Theorem 1.

7.2 Proof of Theorem 2

For any $s > 0$, by Jensen's inequality,

$$\exp(skR_S(F)) = \exp\left(2s\mathbb{E}_\sigma \sup_{f \in F} \sum_{i=1}^{k} \sigma_i f(s_i) \right)$$

$$\leq \mathbb{E}_\sigma \exp\left(2s \sup_{f \in F} \sum_{i=1}^{k} \sigma_i f(s_i) \right)$$

$$\leq \mathbb{E}_\sigma \sum_{f \in F} \exp\left(2s \sum_{i=1}^{k} \sigma_i f(s_i) \right).$$

By Hoeffding's Lemma [20],

$$\mathbb{E}_\sigma \sum_{f \in F} \exp\left(2s \sum_{i=1}^{k} \sigma_i f(s_i) \right)$$

$$\leq \sum_{f \in F} \prod_{i=1}^{k} \exp\left(2s^2 f(s_i)^2 \right)$$

$$= \sum_{f \in F} \exp\left(2s^2 \sum_{i=1}^{k} f(s_i)^2 \right).$$

Let $\ell^2 = \sup_{f \in F} \sum_{i=1}^{k} f(s_i)^2$, and then

$$\sum_{f \in F} \exp\left(2s^2 \sum_{i=1}^{k} f(s_i)^2 \right) \leq |F| \exp\left(2s^2 \ell^2 \right).$$

Thus

$$R_S(F) \leq \frac{1}{sk} (\log |F| + 2s^2 \ell^2),$$

for any $s > 0$. It turns out that to minimize the right hand side of the above equation, we have

$$s = \sqrt{\frac{\log |F|}{2\ell^2}}.$$

Then

$$R_S(F) \leq \frac{\ell}{k} \sqrt{8 \log |F|}.$$

7.3   Discussions of Theorem 3

Theorem 3 can be treated as a special case of Theorem 1 when $m = c$. All the reasoning will not be affected and thus the desired bound follows.