# Approximating All-Pairs Similarity Search by Rademacher Average

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### 1 Introduction

All-pairs similarity search (APSS) has received extensive research interest recently [5, 22, 1, 21]. To improve performance, many approximation approaches have been proposed [10, 8, 12, 7]. This paper considers two approximation methods for cosine similarity based search [20, 22, 1, 21], and SimRank based search [13, 15, 9, 14] respectively. The approximation error of each our algorithm is upper bounded by using Rademacher average [4, 18, 3].

### 2 Problem Formulation and Preliminaries

### 2.1 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  $O(n^2m)$ . Fortunately, there are many methods to detect dissimilar pairs (two vectors without sharing any feature) [1, 21, 16], 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.

#### 2.2 SimRank

SimRank [13] 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 [13]. 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 reverse 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.

### 2.3 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  $v_1, v_2, \dots, v_n$ . 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:  $D = \{1, 2, \dots, m\}$ . 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 [19] 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 [18, 4, 19] 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  $\sigma_i$  is a random variable uniformly distributed over  $\{-1,1\}$ , and the mean  $\mathbb{E}_{\sigma}$  takes randomness over all the  $\sigma_i$ '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

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

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

### Theorem 2.

$$R_S(F) \le \frac{\ell}{k} \sqrt{8\log|F|},$$

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.

# 3 Approximating Cosine Similarities

The approximation algorithm takes as input a collection of n vectors V and two parameters  $(\epsilon, \delta)$  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  $(\epsilon,\delta)$ - 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  $\epsilon$ . Each vector in V contains m features. We take the m features as the sample space  $D = \{1, \dots, m\}$ . 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

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

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

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:

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

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

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

# 4 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 [0,1]. Algorithm 1 shows how to generate a random walk given a sample from  $[0,1]^T$  and a starting

### Algorithm 1 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.
```

node a. It is clear that the random walk chosen by Algorithm 1 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 \le j \le 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

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

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 [0,1]. With probability at least  $1 - \delta$ , we have

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

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:

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

where  $\ell = \max_{f \in F} \sum_{i=1}^k f(s_i)^2$ , 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  $(\epsilon, \delta)$  cannot be satisfied by our algorithm.

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

### References

- [1] Maha Alabduljalil, Xun Tang, and Tao Yang. Cache-conscious performance optimization for similarity search. In *Proceedings of the 36th international ACM SIGIR conference on Research and development in information retrieval*, pages 713–722. ACM, 2013.
- [2] Davide Anguita, Alessandro Ghio, Luca Oneto, and Sandro Ridella. A deep connection between the vapnik–chervonenkis entropy and the rademacher complexity. *IEEE transactions on neural networks and learning systems*, 25(12):2202–2211, 2014.
- [3] Peter L Bartlett, Olivier Bousquet, and Shahar Mendelson. Local rademacher complexities. *Annals of Statistics*, pages 1497–1537, 2005.
- [4] Peter L Bartlett and Shahar Mendelson. Rademacher and gaussian complexities: Risk bounds and structural results. *Journal of Machine Learning Research*, 3(Nov):463–482, 2002.
- [5] Roberto J Bayardo, Yiming Ma, and Ramakrishnan Srikant. Scaling up all pairs similarity search. In *Proceedings of the 16th international conference on World Wide Web*, pages 131–140. ACM, 2007.
- [6] S Boucheron, G Lugosi, and Pascal Massart. A sharp concentration inequality with applications. Random Structures and Algorithms, 1999.
- [7] Moses S Charikar. Similarity estimation techniques from rounding algorithms. In *Proceedings of the thiry-fourth annual ACM symposium on Theory of computing*, pages 380–388. ACM, 2002.
- [8] Ronald Fagin, Ravi Kumar, and Dandapani Sivakumar. Efficient similarity search and classification via rank aggregation. In *Proceedings of the 2003 ACM SIGMOD international conference on Management of data*, pages 301–312. ACM, 2003.
- [9] Yasuhiro Fujiwara, Makoto Nakatsuji, Hiroaki Shiokawa, and Makoto Onizuka. Efficient search algorithm for simrank. In *Data Engineering (ICDE)*, 2013 IEEE 29th International Conference on, pages 589–600. IEEE, 2013.
- [10] Aristides Gionis, Piotr Indyk, Rajeev Motwani, et al. Similarity search in high dimensions via hashing. *VLDB*, 99(6):518–529, 1999.
- [11] Wassily Hoeffding. Probability inequalities for sums of bounded random variables. *Journal of the American statistical association*, 58(301):13–30, 1963.
- [12] Piotr Indyk and Rajeev Motwani. Approximate nearest neighbors: towards removing the curse of dimensionality. In Proceedings of the thirtieth annual ACM symposium on Theory of computing, pages 604–613. ACM, 1998.
- [13] Glen Jeh and Jennifer Widom. Simrank: a measure of structural-context similarity. In *Proceedings* of the eighth ACM SIGKDD international conference on Knowledge discovery and data mining, pages 538–543. ACM, 2002.
- [14] Mitsuru Kusumoto, Takanori Maehara, and Ken-ichi Kawarabayashi. Scalable similarity search for simrank. In *Proceedings of the 2014 ACM SIGMOD international conference on Management of data*, pages 325–336. ACM, 2014.

- [15] Cuiping Li, Jiawei Han, Guoming He, Xin Jin, Yizhou Sun, Yintao Yu, and Tianyi Wu. Fast computation of simrank for static and dynamic information networks. In *Proceedings of the 13th International Conference on Extending Database Technology*, pages 465–476. ACM, 2010.
- [16] Jimmy Lin. Brute force and indexed approaches to pairwise document similarity comparisons with mapreduce. In *Proceedings of the 32nd international ACM SIGIR conference on Research and development in information retrieval*, pages 155–162. ACM, 2009.
- [17] Colin McDiarmid. On the method of bounded differences. Surveys in combinatorics, 141(1):148–188, 1989.
- [18] Mehryar Mohri and Afshin Rostamizadeh. Rademacher complexity bounds for non-iid processes. In Advances in Neural Information Processing Systems, pages 1097–1104, 2009.
- [19] Luca Oneto, Alessandro Ghio, Davide Anguita, and Sandro Ridella. An improved analysis of the rademacher data-dependent bound using its self bounding property. *Neural Networks*, 44:107–111, 2013.
- [20] Alexander Strehl, Joydeep Ghosh, and Raymond Mooney. Impact of similarity measures on web-page clustering. In Workshop on Artificial Intelligence for Web Search (AAAI 2000), pages 58–64, 2000.
- [21] Xun Tang, Maha Alabduljalil, Xin Jin, and Tao Yang. Load balancing for partition-based similarity search. In *Proceedings of the 37th international ACM SIGIR conference on Research & development in information retrieval*, pages 193–202. ACM, 2014.
- [22] Zhihua Xia, Xinhui Wang, Xingming Sun, and Qian Wang. A secure and dynamic multi-keyword ranked search scheme over encrypted cloud data. *IEEE Transactions on Parallel and Distributed Systems*, 27(2):340–352, 2016.

# 5 Appendix

### 5.1 Proof of Theorem 1

In this section, we show our main result (Theorem 1). We start from the definition of self bounding function [19].

**Definition 1.** Let  $s_1, s_2, \dots, s_k$  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  $s_1, \dots, s_{j-1}, s_{j+1}, \dots, s_k \in D$ , the following conditions hold:

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

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

The following concentration inequality can be achieved for self bounding functions [6].

**Lemma 1.** [6] If a function  $Z = f(s_1, \dots, s_k)$  is a self-bounding function with constant c, then for  $t \leq \mathbb{E}Z$ ,

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

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

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  $s_1, s_2, \dots, s_k$ .

*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:

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

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  $Z - G_j \le 2m/k = c$ :

$$G_{j} = \mathbb{E}_{\sigma} \sup_{f \in F} \left[ \frac{2}{k} \sum_{i=1}^{k} \sigma_{i} f(s_{i}) - \frac{2}{k} \sigma_{j} f(s_{j}) \right]$$

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

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

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

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

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

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

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:  $s'_1, \dots, s'_k$  and then we have

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

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.,

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

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

$$\mathbb{E}\sup_{f\in F}\frac{1}{k}\sum_{i=1}^{k}\left[\sigma_{i}(f(s_{i})-f(s_{i}'))\right]\leq 2\mathbb{E}\sup_{f\in F}\frac{1}{k}\sum_{i=1}^{k}\sigma_{i}f(s_{i})=\mathbb{E}R_{S}(F),$$

we have shown the first inequality. The second inequality is analogous.

We also need McDiarmid's inequality [17].

**Lemma 4.** [17] Let  $s_1, \dots, s_k$  be independent random variables taking values from a set D. Suppose a function  $h: D^k \to \mathbb{R}$  satisfies

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

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

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

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

Lemma 5.

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

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

*Proof.* First by Lemma 3,

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

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

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

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

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

It is clear that

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

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

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

By McDiarmid's inequality,

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

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

By Lemma 2,

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

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

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

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

Similarly one can show

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

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

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

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

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

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

Or equivalently,

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

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

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

We have shown Theorem 1.

### 5.2 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 [11],

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

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

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

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

$$\exp(skR_S(F)) \le |F| \exp\left(2s^2\ell^2\right).$$

Let

$$s = \frac{kR_S(F)}{4\ell^2}.$$

Then

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

## 5.3 Discussions of Theorem 3

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