A Tight Lower Bound for Uniformly Stable Algorithms

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Abstract

Leveraging algorithmic stability to derive sharp generalization bounds is a classic and powerful approach in learning theory. Since Vapnik and Chervonenkis [1974] first formalized the idea for analyzing SVMs, it has been utilized to study many fundamental learning algorithms (e.g., k-nearest neighbors [Rogers and Wagner, 1978], stochastic gradient method [Hardt et al., 2016], linear regression [Maurer, 2017], etc.). In a recent line of great works by Feldman and Vondrak [2018, 2019] and Bousquet et al. [2020b], they prove a high probability generalization upper bound of order $\tilde{O}(\gamma + L\sqrt{n})$ for any uniformly $\gamma$-stable algorithm and $L$-bounded loss function. Although much progress was achieved in proving generalization upper bounds for stable algorithms, our knowledge of lower bounds is rather limited. In fact, there is no nontrivial lower bound known ever since the study on uniform stability began [Bousquet and Elisseeff, 2002], to the best of our knowledge. In this paper we fill the gap by proving a tight generalization lower bound of order $\Omega(\gamma + \frac{L}{\sqrt{n}})$, which matches the best known upper bound up to logarithmic factors.

1 Introduction

Estimating the generalization error of learning algorithms is at the heart of modern statistical learning theory. One classic approach is to control the generalization error via notions of model complexity, which has been extensively studied for decades [Vapnik, 2013]. However, as the saying goes "It’s hard to please all", analysis of model complexity doesn’t always give satisfactory answers to all learning algorithms. For example, when analyzing stochastic gradient descent on convex Lipschitz functions, one cannot obtain meaningful generalization bounds by proving uniform convergence for all empirical risk minimizers [Shalev-Shwartz et al., 2010, Feldman, 2016].

Another classic way for proving generalization bounds is to utilize the stability of algorithms, pioneered by Vapnik and Chervonenkis [1974], Rogers and Wagner [1978], Devroye and Wagner [1979a,b] and further studied in Lugosi and Pawlak [1994], Bousquet and Elisseeff [2002], Mukherjee et al. [2006], Shalev-Shwartz et al. [2010], Hardt et al. [2016], Maurer [2017], etc. Intuitively, stability measures the sensitivity of a learning algorithm to the change of a single data point in the training set. Stronger stability often guarantees better generalization as the learning algorithm is robust to small perturbation of data.

In this paper, we study the generalization error of uniformly stable algorithms which were first introduced by Bousquet and Elisseeff [2002]. Formally, we consider the following learning problem

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where we are given a training set $\mathcal{S} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ consisting of $n$ i.i.d. samples from some unknown distribution $\mathcal{D}$ on domain $\mathcal{Z} \subset \mathcal{X} \times \mathcal{Y}$. A learning algorithm $\mathcal{A} : \mathcal{Z}^n \to \mathcal{Y}^n$ is a function which maps a training set to a function mapping from instance space $\mathcal{X}$ into label space $\mathcal{Y}$. We denote by $\mathcal{A}_\mathcal{S} \in \mathcal{Y}^n$ the output function mapping obtained by feeding algorithm $\mathcal{A}$ with training set $\mathcal{S}$.

We measure the performance of $\mathcal{A}_\mathcal{S}$ by a non-negative loss function $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$, and define its population risk as

$$R_{\text{pop}}(\mathcal{A}_\mathcal{S}) = \mathbb{E}_{(x,y) \sim \mathcal{D}} [\ell(\mathcal{A}_\mathcal{S}(x), y)],$$

(1)

as well as its empirical risk as

$$R_{\text{emp}}(\mathcal{A}_\mathcal{S}) = \frac{1}{n} \sum_{i=1}^{n} \ell(\mathcal{A}_\mathcal{S}(x_i), y_i).$$

(2)

One classic approach to control the generalization error $R_{\text{pop}}(\mathcal{A}_\mathcal{S}) - R_{\text{emp}}(\mathcal{A}_\mathcal{S})$ is by restricting the sensitivity of algorithm $\mathcal{A}$ to changes in training set $\mathcal{S}$ (e.g., removing or modifying one of the data points). In order to quantify the sensitivity of algorithms, Vapnik and Chervonenkis [1974], Bousquet and Elisseeff [2002] developed the notion of stability. Formally, a learning algorithm $\mathcal{A}$ is called uniformly $\gamma$-stable (we will use 'stable' as a shorthand for 'uniformly stable' throughout this paper) [Bousquet and Elisseeff, 2002] if for any $\mathcal{S} = \{(x_1, y_1), \ldots, (x_n, y_n)\} \in (\mathcal{X} \times \mathcal{Y})^n$, $\mathcal{S}' = \{(x_1, y_1), \ldots, (x_{i-1}, y_{i-1}), (x_i', y_i'), (x_{i+1}, y_{i+1}), \ldots, (x_n, y_n)\} \in (\mathcal{X} \times \mathcal{Y})^n$ and any $(x, y) \in \mathcal{X} \times \mathcal{Y}$, we have

$$|\ell(\mathcal{A}_\mathcal{S}(x), y) - \ell(\mathcal{A}_\mathcal{S'}(x), y)| \leq \gamma.$$ 

(3)

Many generalization bounds have been proved utilizing the notion of stability (e.g., [Bousquet and Elisseeff, 2002, Feldman and Vondrak, 2018, 2019, Bousquet et al., 2020b]) and the best one is given by Bousquet et al. [2020b]. Specifically, Bousquet et al. [2020b] prove a general moment inequality and use it as a tool to derive a sharp $O(\gamma \log n \log \frac{1}{\delta} + \frac{L}{\sqrt{n}} \sqrt{\log \frac{1}{\delta}})$ bound for any $\gamma$-stable algorithm and $L$-bounded loss function. They also provide an almost matching lower bound for the moment inequality. However, it remains unclear whether this moment lower bound can further imply a lower bound for generalization error.

Although much progress has been achieved in proving generalization upper bounds for stable algorithms, our knowledge of lower bounds is rather limited. In fact, there is no nontrivial lower bound known ever since the study on uniform stability began [Bousquet and Elisseeff, 2002], to the best of our knowledge. In this paper we fill the gap by proving a tight generalization lower bound of order $\Omega(\gamma + \frac{L}{\sqrt{n}})$, which matches the best known upper bound up to logarithmic factors.

**Theorem 1.1** (informal). *There exist domain $\mathcal{X} \times \mathcal{Y}$, distribution $P$ over $\mathcal{X} \times \mathcal{Y}$, $L$-bounded loss function $\ell$, and $\gamma$-stable algorithm $\mathcal{A}$ such that with constant probability over the random drawing of $\mathcal{S}$, the output function mapping $\mathcal{A}_\mathcal{S}$ has generalization error $\Omega(\gamma + \frac{L}{\sqrt{n}})$.*

To the best of our knowledge, Theorem 1.1 provides the first nontrivial and almost matching generalization lower bound for uniformly stable algorithms and therefore deepens our understanding of the methodology of algorithmic stability.

### 1.1 Review of upper bounds

In the seminal work by Bousquet and Elisseeff [2002], they provide the first generalization upper bound that holds for any $\gamma$-stable algorithm and $L$-bounded loss function. Specifically, they prove that with probability at least $1 - \delta$,

$$R_{\text{pop}}(\mathcal{A}_\mathcal{S}) - R_{\text{emp}}(\mathcal{A}_\mathcal{S}) = O\left(\sqrt{n}\gamma \sqrt{\log \frac{1}{\delta} + \frac{L}{\sqrt{n}} \sqrt{\log \frac{1}{\delta}}} \right).$$

(4)
However, its dependence on $n$ is suboptimal in that its tightness is guaranteed only when $\gamma = O(\frac{1}{n})$. This upper bound was recently improved by Feldman and Vondrak [2018, 2019] which show

$$R_{\text{pop}}(A_S) - R_{\text{emp}}(A_S) = O \left( \gamma (\log n)^2 + \gamma \log n \log \frac{1}{\delta} + \frac{L}{\sqrt{n}} \sqrt{\log \frac{1}{\delta}} \right).$$

(5)

The improvement is significant because they remove the $\sqrt{n}$ term so that the rate is optimal as long as $\gamma = O(\frac{1}{\sqrt{n}})$. In the latest work by Bousquet et al. [2020b], this upper bound was further sharpened to

$$R_{\text{pop}}(A_S) - R_{\text{emp}}(A_S) = O \left( \gamma \log n \log \frac{1}{\delta} + \frac{L}{\sqrt{n}} \sqrt{\log \frac{1}{\delta}} \right),$$

(6)

which removes the unnecessary $O(\gamma (\log n)^2)$ term in (5) with a simpler proof. In Bousquet et al. [2020b], they prove a general moment inequality for weakly correlated random variables, and derive (6) as a corollary.

### 1.2 Other related works

The notion of stability was first used in analyzing hard-margin SVMs [Vapnik and Chervonenkis, 1974], which was later followed by Rogers and Wagner [1978], Devroye and Wagner [1979b,a] to prove generalization bounds for $k$-nearest neighbors. Other early works mostly focus on specific learning problems by extending their techniques [Devroye et al., 2013]. Bousquet and Elisseeff [2002] first proved general results on the relationship between stability and generalization, in which they introduced the notion of uniform stability and provided various generalization bounds based on different notions of stability.

As for recent studies on stability, Hardt et al. [2016] proved generalization bounds for stochastic gradient descent using uniform stability. Maurer [2017] studied linear regression with a strongly convex regularizer and a sufficiently smooth loss function. Bousquet et al. [2020a] proved tight exponential upper bounds for the SVM in the realizable setting. And Shalev-Shwartz et al. [2010] proved that by adding a strongly convex term to the objective, ERM solutions to convex learning problems can be made uniformly stable.

Uniform stability also has close relationship with differential privacy [Dwork, 2008]. For example, a differentially private learning algorithm can be reduced to a uniformly stable one by adding noise to the output [Dwork and Feldman, 2018].

### 2 Preliminaries

While various concentration arguments play a vital role in proving upper bounds, to construct hard cases for lower bounds we will need anti-concentration instead. In this section, we introduce some basic anti-concentration inequalities that will be used in our proof.

**Lemma 2.1 (Paley–Zygmund inequality).** Let $Z \geq 0$ be a random variable with bounded second moment. For all $\theta \in [0, 1]$, we have

$$\mathbb{P}(Z > \theta \mathbb{E}(Z)) \geq (1 - \theta)^2 \frac{\mathbb{E}[Z]^2}{\mathbb{E}[Z^2]}.$$  

(7)

**Proof.** We decompose $\mathbb{E}[Z]$ as

$$\mathbb{E}[Z] = \mathbb{E}[Z \times 1_{Z \leq \theta \mathbb{E}[Z]}] + \mathbb{E}[Z \times 1_{Z > \theta \mathbb{E}[Z]}].$$

(8)
The first term is upper bounded by $\theta \mathbb{E}[Z]$, and the second term is at most $\sqrt{\mathbb{E}[Z^2] \mathbb{P}(Z > \theta \mathbb{E}[Z])}$ by Cauchy–Schwarz inequality. The desired inequality thus follows. \hfill \Box

Paley–Zygmund inequality implies that if a non-negative random variable has relatively small variance (so that its standard deviation and mean are of the same order), then with constant probability the random variable and its mean are within the same order of magnitude. Below we utilize Paley–Zygmund inequality to prove an anti-concentration inequality for sum of Rademacher random variables.

**Lemma 2.2** (anti-concentration of sum of Rademacher random variables). Let $X_1, \ldots, X_n$ be independent Rademacher random variables. Then

$$\mathbb{P}\left(\sum_{i=1}^{n} X_i > \frac{\sqrt{n}}{2}\right) \geq \frac{3}{32}.$$  \hfill (9)

**Proof.** Define $S = \sum_{i=1}^{n} X_i$. We have that $\forall i \neq j$

$$\mathbb{E}[X_i^2] = \mathbb{E}[X_i^4] = \mathbb{E}[X_i^2 X_j^2] = 1, \quad \mathbb{E}[X_i X_j] = \mathbb{E}[X_i^3 X_j] = 0.$$  \hfill (10)

Therefore $\mathbb{E}[S^2] = n$ and $\mathbb{E}[S^4] = n + 3n(n - 1) \leq 3n^2$. By Paley–Zygmund inequality (Lemma 2.1), we have $\mathbb{P}(S^2 > n/4) \geq 3/16$. Noting that the distribution of $S$ is symmetric, we conclude $\mathbb{P}(S > \sqrt{n}/2) \geq 3/32$. \hfill \Box

Lemma 2.2 shows that the sum of $n$ independent Rademacher random variables has absolute value $\Omega(\sqrt{n})$ with constant probability. This lemma will play an important role in establishing the $\frac{L}{\sqrt{n}}$ term in our lower bound.

## 3 Main Result

In this section, we present our main result which constructs a hard case such that with constant probability, the $\gamma$-stable learning algorithm $A$ we design has generalization error of order $\Omega(\gamma + \frac{L}{\sqrt{n}})$, which matches the best known upper bound in (6) up to logarithmic factors.

**Theorem 3.1** (lower bound). For any $0 < \gamma \leq L$ and $n \in \mathbb{N}$, there exist domain $\mathcal{X} \times \mathcal{Y}$, distribution $P$ over $Z \subset \mathcal{X} \times \mathcal{Y}$, $L$-bounded loss function $\ell$, and $\gamma$-stable algorithm $A$ such that given a training set $S$ consisting of $n$ i.i.d. samples from $P$, with probability at least $3/64$,

$$R_{\text{pop}}(A_S) - R_{\text{emp}}(A_S) \geq \frac{\gamma}{4} + \frac{L}{32 \sqrt{n}}.$$  \hfill (11)

**Proof.** At a high level, we construct $\mathcal{X}$ to be the collection of base vectors in $\mathbb{R}^d$ where $d \gg n$ and $P$ being the uniform distribution, so that with high probability $S$ samples vectors vertical to each other. We then add a negative copy of each vector and construct $A$ to be a ‘$\gamma$ majority vote’ so that $A$ is as poor as random guess on population, but performs slightly better than random guess on $S$ which brings a $\Omega(\gamma)$ gap in generalization error. Then we extend half of the vectors’ length by twice, so that by using an anti-concentration bound, with constant probability $S$ samples $\Omega(\sqrt{n})$ more ‘shorter’ vectors, which further decreases $R_{\text{emp}}$ by $\Omega(\frac{L}{\sqrt{n}})$.

To begin with, we introduce the construction of our hard case. Given sample size $n$, sensitivity parameter $\gamma > 0$ and boundedness parameter $L \geq \gamma$, we set $d := 4n^2$ and construct

$$\mathcal{X} := \{L\sigma_1 e_1, -L\sigma_1 e_1, \ldots, L\sigma_d e_d, -L\sigma_d e_d\},$$  \hfill (12)
where \( \sigma_i = 1 + I[i > 4] \). Furthermore, let \( \mathcal{Y} := \mathcal{X} \) and \( \mathcal{Z} := \{(x, x) | x \in \mathcal{X}\} \) so that the label \( y \) of each \( x \in \mathcal{X} \) is itself. We choose \( P \) to be the uniform distribution over \( \mathcal{Z} \), and use the \( \ell_1 \)-norm loss function, i.e., \( \ell(y, \hat{y}) := ||y - \hat{y}||_1 \).

Given training set \( \mathcal{S} := \{(x_1, y_1), ... , (x_n, y_n)\} \), our learning algorithm is defined as

\[
\mathcal{A}_S(\pm L \sigma_i e_i) := \text{sign} \left( \left( \sum_{j=1}^{n} x_j \right)_i \right) \gamma \sigma_i e_i, \quad (13)
\]

where \((z)_i\) denotes the \( i \)th coordinate of \( z \). It is easy to check that our learning algorithm \( \mathcal{A} \) is \( 4\gamma \)-stable, and the loss function \( \ell \) is upper bounded by \( 4L \) over \( \mathcal{Y} \times \mathcal{Y} \).

In the remainder of this section, we will prove the generalization error of algorithm \( \mathcal{A} \) is lower bounded by \( \Omega(\gamma + \frac{L}{\sqrt{n}}) \) with constant probability. Specifically, the proof consists of two parts, where the first part aims to compute the population loss \( R_{\text{pop}}(\mathcal{A}_S) \) exactly, and the second one provides an upper bound for the empirical (training) loss \( R_{\text{emp}}(\mathcal{A}_S) \).

**Part 1: compute \( R_{\text{pop}}(\mathcal{A}_S) \) exactly**

We observe that

\[
R_{\text{pop}}(\mathcal{A}_S) = \mathbb{E}_{(x, y) \sim \mathcal{D}} [\ell(\mathcal{A}_S(x), y)] = \frac{1}{2d} \sum_{i=1}^{d} (\| \mathcal{A}_S(L \sigma_i e_i) - L \sigma_i e_i \|_1 + \| \mathcal{A}_S(-L \sigma_i e_i) + L \sigma_i e_i \|_1).
\]

Notice \( \mathcal{A}_S(-L \sigma_i e_i) \equiv \mathcal{A}_S(L \sigma_i e_i) \) always lies on the line segment between \( L \sigma_i e_i \) and \( -L \sigma_i e_i \) by the definition of \( \mathcal{A} \) and \( \gamma \leq L \). As a result, we have

\[
\| \mathcal{A}_S(L \sigma_i e_i) - L \sigma_i e_i \|_1 + \| \mathcal{A}_S(-L \sigma_i e_i) + L \sigma_i e_i \|_1 = 2L \sigma_i,
\]

which directly implies

\[
R_{\text{pop}}(\mathcal{A}_S) \equiv \frac{3L}{2}.
\]  

**Part 2: upper bound \( R_{\text{emp}}(\mathcal{A}_S) \)**

To proceed, we define two useful events: event \( E_1 \) that any two different \( x_i, x_j \) in \( \mathcal{S} \) are orthogonal to each other, and event \( E_2 \) that there are at least \( \sqrt{n}/2 \) more \( x_i \)'s with norm \( L \) than those with norm \( 2L \) in \( \mathcal{S} \). For notational convenience, we further define \( \sigma^{(i)} := ||x_i||_1/L \).

Conditioning on \( E_1 \), we have

\[
R_{\text{emp}}(\mathcal{A}_S) = \frac{1}{n} \sum_{(x, y) \in \mathcal{S}} \ell(\mathcal{A}_S(x), y) = \frac{L - \gamma}{n} \sum_{i=1}^{n} \sigma^{(i)}.
\]  

On the other hand, conditioning on \( E_2 \), we have

\[
\frac{1}{n} \sum_{i=1}^{n} \sigma^{(i)} \leq \frac{1}{n} \mathbb{E} \left[ \sum_{i=1}^{n} \sigma^{(i)} \right] - \frac{1}{8\sqrt{n}} = \frac{3}{2} - \frac{1}{8\sqrt{n}}.
\]  

Combining equations (14), (15) and (16), we obtain the desired lower bound

\[
R_{\text{emp}}(\mathcal{A}_S) = \frac{L - \gamma}{n} \sum_{i=1}^{n} \sigma^{(i)} \leq (L - \gamma) \left( \frac{3}{2} - \frac{1}{8\sqrt{n}} \right) \leq R_{\text{pop}}(\mathcal{A}_S) - \frac{L}{8\sqrt{n}} - \gamma.
\]
Now, the only thing left is to estimate $\mathbb{P}(E_1 \cap E_2)$. By Lemma 2.2, we have $\mathbb{P}(E_2) \geq 3/32$. Moreover, note that
\[
\mathbb{P}(E_1 | E_2) \geq (1 - \frac{n}{0.5d})^n = \left(1 - \frac{1}{2n}\right)^n \geq 1 - \frac{1}{2} = \frac{1}{2}.
\]
Therefore, we obtain $\mathbb{P}(E_1 \cap E_2) = \mathbb{P}(E_1 | E_2) \mathbb{P}(E_2) \geq 3/64$. Finally, rescaling $\gamma$ and $L$ by $1/4$ concludes the whole proof.

**Remark 3.2.** We can also avoid analyzing the relationship between events $E_1$ and $E_2$ by setting $d$ large enough and taking a union bound on $\neg E_1$ and $\neg E_2$.

Theorem 3.1 directly implies that it is impossible to achieve $o(\gamma + \frac{L}{\sqrt{n}})$ generalization error and the upper bound in [Bousquet et al., 2020b] is almost optimal. We comment that our lower bound here holds with constant probability and it would be interesting to generalize it to the high-probability regime so that it can reveal the dependence on the failure probability. And to do that, the first step might be to replace Lemma 2.2 with a stronger anti-concentration inequality that can handle relatively small probability $\delta \ll 1$.

4 Conclusion

In this paper we prove a tight $\Omega(\gamma + \frac{L}{\sqrt{n}})$ generalization lower bound for uniformly stable algorithms, which matches the best known upper bound in [Bousquet et al., 2020b] up to logarithmic factors. To the best of our knowledge, this result provides the first matching lower bound which has been unknown for more than a decade since the first upper bound was given in [Bousquet and Elisseeff, 2002], thus greatly complementing our knowledge about the limit of this classic framework.

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