On the Stability of Empirical Risk Minimization in the Presence of Multiple Risk Minimizers

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Abstract—Recently Kutin and Niyogi investigated several notions of algorithmic stability—a property of a learning map conceptually similar to continuity—showing that training-stability is sufficient for consistency of Empirical Risk Minimization while distribution-free CV-stability is necessary and sufficient for having finite VC-dimension. This paper concerns a phase transition in the training stability of ERM, conjectured by the same authors. Kutin and Niyogi proved that ERM on finite hypothesis spaces containing a unique risk minimizer has training stability that scales exponentially with sample size, and conjectured that the existence of multiple risk minimizers prevents even super-quadratic convergence. We prove this result for the strictly weaker notion of CV-stability, positively resolving this conjecture for weaker CV-stability and stable for no minimizers, for example when learning in a symmetric hypothesis class with positive minimum risk. Results showing poor generalization in such cases, as implied by slow rates of stability, help to justify the use of feature selection. It is also noteworthy that restricting focus to finite hypothesis classes is far from unreasonable—practitioners often attempt to learn on extracted features, which frequently involves discretization, and when learning on a finite domain any hypothesis space becomes effectively finite.

II. PRELIMINARIES

We follow the setting of [5] closely. \( X \) denotes the input space, \( Y = \{-1, 1\} \) the output space and \( Z = X \times Y \) their product example space. \( D \) is a distribution on \( Z \). Unless stated otherwise we assume that \( m \) examples are drawn i.i.d. according to \( D \). A classifier or hypothesis is a function \( h : X \to \{-1, 1\} \); \( \mathcal{H} \) denotes a set of classifiers or a hypothesis space. Whenever we refer to a finite \( \mathcal{H} \) we assume, without loss of generality, that no \( h_1, h_2 \in \mathcal{H} \) exist such that \( h_1 \neq h_2 \) and \( h_1(X) = h_2(X) \) a.s.

A learning algorithm on hypothesis space \( \mathcal{H} \) is a function \( A : \bigcup_{m>0} \mathbb{Z}^m \to \mathcal{H} \). When \( A \) is understood from the context, we write \( f_s = A(s) \) for \( s \in \mathbb{Z}^m \). The loss incurred by classifier \( h \) on example \( z \in Z \) is denoted by \( \ell(h, z) \). We will assume the 0-1 loss throughout, where \( \ell(h, (x, y)) = 1 \) if \( h(x) \neq y \). Define the risk of \( h \) with respect to \( D \) as \( R_D(h) = \mathbb{E}_{Z \sim D} \ell(h, Z) \); and with a slight abuse of notation the empirical risk as \( R_s(h) = m^{-1} \sum_{i=1}^m \ell(h, z_i) \) for \( s = (z_1, \ldots, z_m) \in \mathbb{Z}^m \). The risk minimizers of \( \mathcal{H} \) with respect to distribution \( D \) is the set \( \mathcal{H}^* = \arg\min_{h \in \mathcal{H}} R_D(h) \).

A learning algorithm \( A \) is said to implement Empirical Risk Minimization if \( A(s) \in \arg\min_{h \in \mathcal{H}} R_s(h) \) for \( s \in \mathbb{Z}^m \). Based on sequence \( s = (z_1, \ldots, z_m) \in \mathbb{Z}^m \), index \( i \in [m] \) and example \( u \in Z \), we define sequences \( s_i = (z_1, \ldots, z_{i-1}, z_{i+1}, \ldots, z_m) \in \mathbb{Z}^{m-1} \) and \( s_i^u = (z_1, \ldots, z_{i-1}, u, z_{i+1}, \ldots, z_m) \in \mathbb{Z}^m \). The following definitions capture the relevant notions of stability.

Definition 2.1: A learning algorithm \( A \) is weakly \((\beta, \delta)\)-hypothesis-stable or has weak hypothesis stability \((\beta, \delta)\) if for any \( i \in [m] \),

\[
\Pr_{(S, U) \sim D^{m+1}} \left( \max_{z \in \mathbb{Z}} |\ell(f_S, z) - \ell(f_{S_i^U}, z)| \leq \beta \right) \geq 1 - \delta.
\]

The notion of weak hypothesis stability was first used by Devroye and Wagner in [3] under the name of stability. Kearns and Ron [4] then used the term hypothesis stability for the same concept.
Definition 2.2: A learning algorithm $A$ is $(\beta, \delta)$-cross-validation-stable, or $(\beta, \delta)$-CV-stable, if, for any $i \in [m],$
\[
\Pr_{(S,U) \sim D^{m+1}}(|\ell(f_S, U) - \ell(f_{S,U}, U)| \leq \beta) \geq 1 - \delta .
\]

Definition 2.3: A learning algorithm $A$ is $(\beta, \delta)$-overlap-stable, or has overlap stability $(\beta, \delta)$, if, for any $i \in [m],$
\[
\Pr_{(S,U) \sim D^{m+1}}(|R_S(f_S) - R_{S,U}(f_{S,U})| \leq \beta) \geq 1 - \delta .
\]

Combining CV and overlap stability, Kutin and Niyogi arrive at the next definition.

Definition 2.4: A learning algorithm $A$ is $(\beta, \delta)$-training-stable or, has training stability $(\beta, \delta)$, if $A$ has
i. CV stability $(\beta, \delta)$; and
ii. Overlap stability $(\beta, \delta)$.

Trivially weak hypothesis stability $(\beta, \delta)$ implies training stability $(\beta, \delta)$. Kutin and Niyogi show that training stability is sufficient for good bounds on generalization error (for ERM, CV stability is sufficient). They also consider the stability of ERM on a two-classifier hypothesis class [5, Theorems 9.2 and 9.5], showing that the achievable rate on $\delta$ undergoes a phase transition as the number of risk minimizers increases from one to two.

Theorem 2.5: Consider the class $H$ consisting of the two constant classifiers mapping $X$ to $-1$ and $1$ respectively, and let $A$ implement ERM on $H$ (i.e., $A$ outputs a majority label of training set $S$). Let $p = Pr(X,Y)D(Y = 1)$. If $p \geq \frac{1}{2}$ then $A$ is $(0, \delta)$-training-stable for $\delta(m) \approx (2\pi m)^{-1/2}$.

2. If $p > \frac{1}{2}$ then $A$ is weakly $(0, \delta)$-hypothesis-stable for $\delta = \exp\left(-\frac{(2 - p)^2}{2} m/8 + O(1)\right)$.

3. If $p = \frac{1}{2}$ then $A$ is not $(\beta, \delta)$-CV-stable, or $(\beta, \delta)$-overlap-stable for any $\beta < 1$ and any $\delta = o(m^{-1/2})$.

The case of finite hypothesis spaces is then considered. In particular the authors show that fast rates are achieved in the presence of a unique risk minimizer.

Theorem 2.6: Let $H$ be a finite collection of classifiers, and let $A$ be a learning algorithm which performs ERM over $H$. Suppose there exists a unique risk minimizer $h^* \in H$, then $A$ is weakly $(0, \delta)$-hypothesis-stable for $\delta = \exp(-\Omega(m))$.

The authors then conjecture that the analogue of Theorem 2.5(3) holds for general $|H| < \infty$: [5, Conjecture 10.11] predicts that under any distribution $D$ inducing multiple risk minimizers, ERM is not $(0, \delta)$-training-stable for any $\delta = o(m^{-1/2})$.

III. Finite Classes with Multiple Risk Minimizers

Lemma 3.1: Let $H$ be a finite hypothesis space with $|H| \geq 2$ and with risk minimizers satisfying $|H^*| = 2$. Then ERM on $H$ with respect to the 0-1 loss, on a sample of $m$ examples, is not $(0, \delta)$-CV-stable for any $\delta = o(m^{-1/2})$. Furthermore, ERM on $H$ is $(0, \delta)$-CV-stable for $\delta = O(m^{-1/2})$.

Proof: Let $H^* = \{h_1, h_2\}$. We proceed by first showing that $f_\delta$ lies in $H^*$ with exponentially increasing probability and then that switching within $H^*$ occurs often. Let $\epsilon = \min_{h \in H^*} R_D(h) - R_D(h_1)$, which exists and is positive by the finite cardinality of $H$. Then by the union bound, $R_D(h) \geq R_D(h_1) + \epsilon$ for all $h \in H \setminus H^*$, and Chernoff’s bound
\[
Pr(f_S \in H^*) \geq Pr(\forall h \in H \setminus H^*, R_S(h_1) < R_S(h)) \geq Pr(\forall h \in H \setminus H^*, R_S(h_1) < R_D(h_1) + \epsilon/2 < R_S(h)) \geq 1 - Pr(R_S(h_1) > R_D(h_1) + \epsilon/2)
\]
\[
= 1 - \sum_{h \in H \setminus H^*} Pr(R_D(h_1) + \epsilon/2 > R_S(h))
\]
\[
\geq 1 - \sum_{h \in H \setminus H^*} Pr(R_D(h) - \epsilon/2 > R_S(h))
\]
\[
\geq 1 - \exp(-\epsilon^2 m/2) = 1 - (|H| - 1) \exp(-\epsilon^2 m/2) .
\]

Consider ERM on $H^*$. Without loss of generality assume that ERM on $H^*$, when $h_1$ and $h_2$ have equal empirical risk, selects $h_1$. Let $Z_1 = \{z \in Z \mid \ell(h_1, z) < \ell(h_2, z)\}$ and $Z_2$ be defined analogously. Let $p = Pr(Z \in Z_1 \cup Z_2)$, which is positive by assumption that $h'(X) = h''(X)$ a.s. implies $h' = h''$. Then for all $i \in [m]$
\[
Pr(|R_S(h_1) - R_S(h_2)| \leq (m - 1)^{-1}) = O\left(m^{-1/2}\right) .
\]

Conditioned on the events of (2) and (3), the probability of ERM on $S$ outputting a different hypothesis than on $S_{i,U}$ is at least 1/2. This fact can be proved by cases on $|R_S(h_1) - R_S(h_2)|$, while assuming that $(Z_i, U) \in (Z_1 \times Z_2) \cup (Z_2 \times Z_1)$. If $R_S(h_1) = R_S(h_2)$, then $f_S \neq f_{S,U}$ trivially. If $R_S(h_1) > R_S(h_2)$, then it follows that $R_S(h_1) - R_S(h_2) = (m - 1)^{-1}$ and since by symmetry the probability that $R_S(x(h_1) > R_S(x(h_2))$ conditioned on the corresponding difference being $2m^{-1}$ is 1/2, it follows that $f_S \neq f_{S,U}$ with probability 1/2. Thus we have shown that on $H^*$, for all $i \in [m]$
\[
Pr(S,U)\sim D^{m+1}(|f_S \neq f_{S,U} | \mathcal{A} \cap \mathcal{B}) \geq 1/2 ,
\]
where
\[
\mathcal{A} = \{(S,U) : (Z_i, U) \in (Z_1 \times Z_2) \cup (Z_2 \times Z_1)\}
\]
\[
\mathcal{B} = \{(S,U) : |R_S(h_1) - R_S(h_2)| \leq (m - 1)^{-1}\} .
\]

Notice that since $f_S, f_{S,U} \in H^*$ and $U \in Z_1 \cup Z_2$, $f_S \neq f_{S,U}$ implies that $\ell(f_S, U) \neq \ell(f_{S,U}, U)$. Then together [1]–[4] lead to the following statement about ERM over $H$:
\[
Pr(S,U)\sim D^{m+1}(|\ell(f_S, U) - \ell(f_{S,U}, U)| > 0)
\]
\[
\geq Pr(|\ell(f_S, U) - \ell(f_{S,U}, U)| > 0, f_S, f_{S,U} \in H^*)
\]
\[
\geq O\left(p^2 m^{-1/2}\right) - 2(|H| - 1) \exp(-\epsilon^2 m/2)\]
\[
= O\left(m^{-1/2}\right) .
\]
And so ERM is not \((0, \delta)-CV\)-stable for any \(\delta = o(m^{-1/2})\) as claimed. Furthermore ERM is \((0, \delta)-CV\)-stable for \(\delta = O(m^{-1/2})\) since
\[
Pr_{(S,U)}[D_m \neq 1]|\ell(f_S, U) - \ell(f_{S\star}, U)\rangle > 0) \\
\leq Pr(|\ell(f_S, U) - \ell(f_{S\star}, U)| > 0, f_S, f_{S\star} \in \mathcal{H}^*) \\
+ Pr(f_S \notin \mathcal{H}^* \lor f_{S\star} \notin \mathcal{H}^*) \\
\leq O\left(m^{-1/2}\right) + 2|\mathcal{H}| \cdot 1 \exp\left(-c^2 m/2\right) \\
= O\left(m^{-1/2}\right).
\]

All that remains is to verify (3). Consider \(X_{m,n,q} \sim Bin(n, q)\) for \(n \in \mathbb{N}, q \in [0, 1]\) and note that for \(k \in \mathbb{N} \cup \{0\}\)
\[
Pr\left(\left|X_{k,\frac{1}{2}} - k \cdot \frac{1}{2}\right| \leq \frac{1}{2}\right) = \begin{cases} \Pr\left(X_{k,\frac{1}{2}} = \frac{k}{2}\right), & k \text{ even} \\ 2\Pr\left(X_{k,\frac{1}{2}} = \frac{k-1}{2}\right), & k \text{ odd} \end{cases} \\
\geq \Pr\left(X_{\frac{m}{2}} \leq k \cdot \frac{1}{2}\right) = \frac{k}{2}.
\]

Splitting on \(\sum_{j=1}^{m} \mathbb{I}\{Z_j \in \mathbb{Z}_1 \cup \mathbb{Z}_2\}\) the Bin \((m-1, p)\) number of examples in \(S^l\) on which \(h_1, h_2\) disagree—and noting that when conditioned on this sum being equal to \(k\), the random variable \(\frac{m-1}{2} (R_S(h_1) - R_S(h_2)) + k \cdot \frac{1}{2} \sim Bin(k, 1/2)\), leads to the lower-bound
\[
Pr\left(|R_S(h_1) - R_S(h_2)| \leq (m-1)^{-1}\right) \\
= \sum_{k=0}^{m-1} \Pr(X_{m-1,p} = k) \Pr\left(|X_{k,\frac{1}{2}} - k \cdot \frac{1}{2}| \leq \frac{1}{2}\right) \\
\geq \min_{0 \leq k \leq m-1} \Pr\left(|X_{k,\frac{1}{2}} - k \cdot \frac{1}{2}| \leq \frac{1}{2}\right) \sum_{j=0}^{m} \Pr(X_{m-1,p} = j) \\
= \min_{0 \leq k \leq m-1} \Pr\left(|X_{\frac{m}{2}} - k \cdot \frac{1}{2}| \leq \frac{1}{2}\right) \\
= \Pr\left(X_{\frac{m}{2}} \leq k \cdot \frac{1}{2}\right) = \frac{m}{2} \\
= O\left(m^{-1/2}\right),
\]
where the last relation is a consequence of Stirling’s approximation. Let \(c = \lfloor p(m-1)/2\rfloor\). The upper-bound follows similarly:
\[
Pr\left(|R_S(h_1) - R_S(h_2)| \leq (m-1)^{-1}\right) \\
= \sum_{k=0}^{m-1} \Pr(X_{m-1,p} = k) \Pr\left(|X_{\frac{m}{2}} - k \cdot \frac{1}{2}| \leq \frac{1}{2}\right) \\
\leq \Pr(X_{m-1,p} \leq c) \\
+ \sup_{k \in \{c+1, \ldots, m-1\}} \Pr\left(|X_{\frac{m}{2}} - k \cdot \frac{1}{2}| \leq \frac{1}{2}\right) \\
\leq O(e^{-pm}) + O\left(m^{-1/2}\right) \\
= O\left(m^{-1/2}\right),
\]
where the penultimate relation follows from an application of Chernoff’s inequality to the first term and Stirling’s approximation to the second.

Theorem 3.2: Let \(\mathcal{H}\) be a finite hypothesis space with \(|\mathcal{H}| \geq 2\) and with risk minimizers \(|\mathcal{H}^*| > 1\). Then any learning algorithm \(\mathcal{A}\) implementing ERM on \(\mathcal{H}\) with respect to the 0-1 loss, on a sample of \(m\) examples, is not \((0, \delta)-CV\)-stable for any \(\delta = o(m^{-1/2})\). Furthermore, \(\mathcal{A}\) is \((0, \delta)-CV\)-stable for \(\delta = O(m^{-1/2})\).

Proof: Define \(c\) as before. Arbitrarily order the risk minimizers \(\mathcal{H}^* = \{h_1, \ldots, h_n\}\) where \(|\mathcal{H}^*| = n\), and let \(p_{ij} = Pr(h_i(X) \neq h_j(X)) > 0\) by assumption that \(h'(X) = h''(X)\) a.s. implies \(h' = h''\) for each \(h, h'' \in \mathcal{H}\). Let \(f_{S,ij}^*\) be the result of running \(\mathcal{A}\) on sample \(T\) in the hypothesis space \(\{h_1, h_2\}\), where ties between empirical risk minimizers are broken as in ERM over \(\mathcal{H}^*\). Let \(f_{T,ij}^*\) be the result of running \(\mathcal{A}\) on \(T\) in \(\mathcal{H}^*\). It follows that for all \(\{j, k\} \subseteq [n]\), conditional upon event \(\mathcal{E}_{jk} = \{f_{S,ij}^* = h_j, f_{S,ik}^* = h_k\}, f_{S,ij}^* = f_{S,ik}^* = f_{S,ik}^* = h_k\) and so by (4)
\[
Pr_{(S,U)}[D_m \neq 1]|\ell(f_S, U) - \ell(f_{S\star}, U)| > 0 | \mathcal{E}_{jk} \\
\geq Pr\left(\ell(f_{S,ij}^*, U) - \ell(f_{S,ik}^*, U) > 0 | \mathcal{E}_{jk}\right) \\
\geq O\left(m^{-1} \min_{(j,k) \subseteq [n]} p_{jk}^2 m^{-1/2}\right). \tag{5}
\]
It follows that
\[
Pr_{(S,U)}[D_m \neq 1]|\ell(f_S, U) - \ell(f_{S\star}, U)| > 0 \geq \min_{(j,k) \subseteq [n]} Pr\left(|\ell(f_S, U) - \ell(f_{S\star}, U)| > 0 | \mathcal{E}_{jk}\right) \\
\geq O\left(m^{-1} \min_{(j,k) \subseteq [n]} p_{jk}^2 m^{-1/2}\right). \tag{6}
\]
Observeing that \(Pr(f_S \in \mathcal{H}^*) \geq 1 - |\mathcal{H}| \cdot \exp(-c^2 m/2)\) by the same argument that lead to (4), we have as before
\[
Pr(|\ell(f_S, U) - \ell(f_{S\star}, U)| > 0) \\
\geq \Pr(|\ell(f_S, U) - \ell(f_{S\star}, U)| > 0, f_S, f_{S\star} \in \mathcal{H}^*) \\
\geq \Pr(|\ell(f_S^*, U) - \ell(f_{S\star}^*, U)| > 0) \\
\times (1 - Pr(f_S \notin \mathcal{H}^* \lor f_{S\star} \notin \mathcal{H}^*)) \\
= O\left(\min_{(j,k) \subseteq [n]} p_{jk}^2 m^{-1/2}\right) (1 - 2|\mathcal{H}| \cdot \exp(-c^2 m/2)) \\
= O\left(m^{-1/2}\right). \tag{7}
\]
This implies that ERM on \(\mathcal{H}\) is not \((0, \delta)-CV\)-stable for any \(\delta = o(m^{-1/2})\). Similarly we derive an upper-bound analogous to (7) by the same technique used in the proof of Lemma 3.1
\[
Pr(|\ell(f_S, U) - \ell(f_{S\star}, U)| > 0) \\
\leq \Pr(|\ell(f_{S\star}, U) - \ell(f_S, U)| > 0, f_S, f_{S\star} \in \mathcal{H}^*) \\
+ Pr(f_S \notin \mathcal{H}^* \lor f_{S\star} \notin \mathcal{H}^*) \\
= O\left(\max_{(j,k) \subseteq [n]} p_{jk}^2 m^{-1/2}\right) + 2|\mathcal{H}| \cdot \exp(-c^2 m/2) \\
= O\left(m^{-1/2}\right).
\]
This implies that ERM on \(\mathcal{H}\) is \((0, \delta)-CV\)-stable for \(\delta = O(m^{-1/2})\). \(\Box\)
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