Sharpened Generalization Bounds based on Conditional Mutual Information and an Application to Noisy, Iterative Algorithms

Mahdi Haghifam\textsuperscript{1,3} Jeffrey Negrea\textsuperscript{2,3} Ashish Khisti\textsuperscript{1} Daniel M. Roy\textsuperscript{2,3} Gintare Karolina Dziugaite\textsuperscript{4}

\textsuperscript{1}Dept. of Electrical and Computer Engineering, University of Toronto
\textsuperscript{2}Dept. of Statistical Sciences, University of Toronto
\textsuperscript{3}Vector Institute for Artificial Intelligence
\textsuperscript{4}Element AI

Abstract

The information-theoretic framework of Russo and J. Zou (2016) and Xu and Raginsky (2017) provides bounds on the generalization error of a learning algorithm in terms of the mutual information between the algorithm’s output and the training sample. In this work, we study the proposal, by Steinke and Zakynthinou (2020), to reason about the generalization error of a learning algorithm by introducing a super sample that contains the training sample as a random subset and computing mutual information conditional on the super sample. We first show that these new bounds based on the conditional mutual information are tighter than those based on the unconditional mutual information. We then introduce yet tighter bounds, building on the “individual sample” idea of Bu, S. Zou, and Veeravalli (2019) and the “data dependent” ideas of Negrea et al. (2019), using disintegrated mutual information. Finally, we apply these bounds to the study of Langevin dynamics algorithm, showing that conditioning on the super sample allows us to exploit information in the optimization trajectory to obtain tighter bounds based on hypothesis tests.

1 Introduction

Let $\mathcal{D}$ be an unknown distribution on a space $\mathcal{Z}$, and let $\mathcal{W}$ be a set of parameters that index a set of predictors with a bounded loss function $\ell : \mathcal{Z} \times \mathcal{W} \to [0, 1]$. Consider a (randomized) learning algorithm $\mathcal{A}$ that selects an element $W$ in $\mathcal{W}$, on the basis of an IID sample $S = (Z_1, \ldots, Z_n) \sim \mathcal{D}^\otimes n$. For $w \in \mathcal{W}$, let $R_{\mathcal{D}}(w) = \mathbb{E}[\ell(Z, w)]$ denote the risk of the predictor indexed by $w$, and let $\hat{R}_S(w) = \frac{1}{n} \sum_{i=1}^{n} \ell(Z_i, w)$ denote the empirical risk. Our primary interest in this paper is the (expected) generalization error of $\mathcal{A}$ with respect to $\mathcal{D}$,

$$\text{EGE}_{\mathcal{D}}(\mathcal{A}) = \mathbb{E}[R_{\mathcal{D}}(W) - \hat{R}_S(W)],$$

averaging over both the choice of dataset and the randomness within $\mathcal{A}$.

In this work, we study bounds on generalization error in terms of information-theoretic measures of dependence between the data and the output of the learning algorithm. This approach was initiated by Russo and J. Zou (2015, 2016) and has since been extended (Raginsky et al., 2016; Xu and Raginsky, 2017; Asadi, Abbe, and Verdù, 2018; Bu, S. Zou, and Veeravalli, 2019). The basic result in this line of work is that the generalization error can be bounded in terms of the mutual information $I(W; S)$ between the data and the learned parameter, a quantity that has been called the information usage or input–output
The mutual information of $A$ with respect to $D$, which we denote by $\text{IOMI}_D(A)$. The following result is due to Russo and J. Zou (2016) and Xu and Raginsky (2017).

**Theorem 1.1.** $\text{EGE}_D(A) \leq \sqrt{\frac{1}{2n} \text{IOMI}_D(A)}$.

Theorem 1.1 formalizes the intuition that a learning algorithm without heavy dependence on the training set will generalize well.

This result has been extended in many directions: Raginsky et al. (2016) connect variants of $\text{IOMI}_D(A)$ to different notions of stability. Asadi, Abbe, and Verdú (2018) establish refined bounds using chaining techniques for subgaussian processes. Bu, S. Zou, and Veeravalli, 2019 obtain a tighter bound by replacing $\text{IOMI}_D(A)$ with the mutual information between $W$ and a single training data point. Negrea et al. (2019) propose variants that allow for data-dependent estimates. See also (Jiao, Han, and Weissman, 2017; A. Lopez and V. Jog, 2018; Bassily et al., 2018).

Our focus in this paper is a new class of information-theoretic bounds on generalization error, proposed by Steinke and Zakynthinou (2020), which we now introduce: Fix $k \geq 2$, let $[k] = \{1, \ldots, k\}$, let $U^{(k)} = (U_1, \ldots, U_n)$ be distributed uniformly in $[k]^n$, and let

$$
\tilde{Z}^{(k)} = \begin{pmatrix} Z_{1,1} & \cdots & Z_{1,n} \\
\vdots & \ddots & \vdots \\
Z_{k,1} & \cdots & Z_{k,n} 
\end{pmatrix}
$$

be an array of IID random elements in $Z$, independent from $U^{(k)}$, with distribution $D$. Put $S = (Z_{U_1,1}, \ldots, Z_{U_n,n})$ and let $W$ be a random element in $W$ satisfying $P_{S, U^{(k)}, Z^{(k)}}(W) = \mathcal{A}(S)$, i.e., conditional on $S$, $U^{(k)}$, and $Z^{(k)}$, $W$ has distribution $\mathcal{A}(S)$. It follows that, conditional on $S$, $W$ is independent from $U^{(k)}$ and $Z^{(k)}$. By construction, the data set $S$ is hidden inside the super sample; the indices $U^{(k)}$ specify where. Steinke and Zakynthinou (2020) make use of these additional structures to define a new information-theoretic notion:

**Definition 1.2** (Steinke and Zakynthinou 2020). The conditional mutual information of $A$ with respect to $D$ is $\text{CMI}_D^k(A) = I(W; U^{(k)} | \tilde{Z}^{(k)})$.

Intuitively, $\text{CMI}_D^k(A)$ captures how well we can recognize which samples from the given super-sample $\tilde{Z}^{(k)}$ were in the training set of the algorithm, given the learned parameters. This intuition can be formalized using Fano’s inequality, showing that $\text{CMI}_D^k(A)$ can be used to lower bound the error of any estimator of $U^{(k)}$ given $W$ and $\tilde{Z}^{(k)}$. (See Appendix A.) Steinke and Zakynthinou connect $\text{CMI}_D^k(A)$ with well-known notions in learning theory such as distributional stability, differential privacy, and VC dimension, and establish the following bound (Steinke and Zakynthinou, 2020, Thm. 5.1), which we state here for general $k \geq 2$, as it is a straightforward extension:

**Theorem 1.3.** $\text{EGE}_D(A) \leq \sqrt{\frac{2}{n} \text{CMI}_D^k(A)}$.

In this paper, we aim to improve our understanding of the framework introduced by Steinke and Zakynthinou (2020), identify tighter bounds, and apply these techniques in the analysis of a realistic algorithm. In Section 2, we present several formal connections between the two aforementioned information-theoretic approaches for studying generalization. Our first result builds a bridge between $\text{IOMI}_D(A)$ and $\text{CMI}_D^k(A)$ by showing that for any learning algorithm, any data distribution, and any $k$, $\text{CMI}_D^k(A)$ is less that $\text{IOMI}_D(A)$. We further show that $\text{CMI}_D^k(A)$ converges to $\text{IOMI}_D(A)$ as $k \to \infty$, for the case where $W$ is a finite set. In Section 3, we establish two novel upper bounds on generalization error using the same index and super sample structure exploited by Steinke and Zakynthinou, and we show that both of our bounds are tighter than the bound based on $\text{CMI}_D^k(A)$. Finally, in Section 4, we provide a general recipe for constructing generalization error bounds for
noisy, iterative algorithms using the generalization bound proposed in Section 3. We then apply this recipe to the particular example of Langevin dynamics algorithm, and show that the obtained generalization bound is tighter than existing information-theoretic bounds for Langevin dynamics algorithm (Pensia, Jog, and Loh, 2018; Bu, S. Zou, and Veeravalli, 2019; Li, Luo, and Qiao, 2020).

### 1.1 Notation

Let $S, T$ be measurable spaces, let $\mathcal{M}_1(S)$ be the space of probability measures on $S$, and define a probability kernel from $S$ to $T$ to be a measurable map from $S$ to $\mathcal{M}_1(T)$. For random elements $X$ in $S$ and $Y$ in $T$, write $\mathbb{P}[X] \in \mathcal{M}_1(S)$ for the distribution of $X$ and write $\mathbb{P}^Y[X]$ for (a regular version of) the conditional distribution of $X$ given $Y$, viewed as a random element in $\mathcal{M}_1(T)$. Recall that $\mathbb{P}^Y[X]$ is a regular version if, for some probability kernel $\kappa$, we have $\mathbb{P}^Y[X] = \kappa(Y)$ a.s. In particular, $\mathbb{P}^Y[X]$ is $Y$-measurable. If $X$ is a random variable (i.e., random element in $\mathbb{R}$ under its standard Borel structure), write $\mathbb{E}X$ for the expectation of $X$ and write $\mathbb{E}^P X$ or $\mathbb{E}[X|Y]$ for (an arbitrary version of) the conditional expectation of $X$ given $Y$, which is $Y$-measurable by definition.

Let $P, Q$ be probability measures on a measurable space $S$. For a $P$-integrable function or nonnegative measurable function $f$, let $P[f] = \int f dP$. When $Q$ is absolutely continuous with respect to $P$, denoted $Q \ll P$, we write $\frac{dQ}{dP}$ for (an arbitrary version of) the Radon–Nikodym derivative (or density) of $Q$ with respect to $P$, satisfying, per the Radon–Nikodym theorem, $Q(A) = P[\{1\} \frac{dQ}{dP}]$, for all measurable subsets $A$, where $\{1\}$ denotes the characteristic function of a set $A$.

We rely on several notions from information theory: The KL divergence (or relative entropy) of $Q$ with respect to $P$, denoted $\text{KL}(Q \| P)$, is $\text{KL}(Q \| P) = \int \log \frac{dQ}{dP}$ when $Q \ll P$ and infinity otherwise. Let $X$, $Y$, and $Z$ be random elements. The mutual information between $X$ and $Y$ is

$$I(X; Y) = \text{KL}(\mathbb{P}[(X, Y)] \| \mathbb{P}[X] \otimes \mathbb{P}[Y]),$$

where $\otimes$ forms the product measure. The disintegrated mutual information between $X$ and $Y$ given $Z$, is

$$I^Z(X; Y) = \text{KL}(\mathbb{P}^Z[(X, Y)] \| \mathbb{P}^Z[X] \otimes \mathbb{P}^Z[Y]).$$

Then the conditional mutual information of $X$ and $Y$ given $Z$ is $I(X, Y | Z) = \mathbb{E}I^Z(X, Y)$.

Let $\mu = \mathbb{P}[X]$ and let $\kappa(Y) = \mathbb{P}^Y[X]$ a.s. If $X$ concentrates on a countable set $S$ with counting measure $\nu$, the (Shannon) entropy of $X$ is $H(X) = -\mathbb{E}\log \frac{d\nu}{d\mathbb{P}} = -\sum_{x \in S} \mathbb{P}(X = x) \log \mathbb{P}(X = x)$, while the conditional entropy of $X$ given $Y$ is $H(X | Y) = -\mathbb{E}[\kappa(Y) \log \frac{d\kappa(Y)}{d\mathbb{P}}]$.

We have $H(X | Y) \leq H(X)$.

For integers $n \geq 1$, let $[n] = \{1, \ldots, n\}$ and, for $k \in [n]$, let $[n]_k$ denote the set of all subsets of $[n]$ of size $k$. For a sequence $X = (X_1, \ldots, X_n)$ and a subset $A \subseteq [n]$, let $X_{A}$ denote the subsequence $(X_i)_{i \in A}$.

### 2 Generalization Guarantees using Mutual Information

In this section, we compare the two approaches to the information-theoretic analysis of generalization error based on mutual information and conditional mutual information. Our main results (Theorems 2.1 and 2.2) show that for any learning algorithm and any data distribution, conditional mutual information provides a tighter measure of dependence than mutual information, and that one can recover the mutual-information–based bounds in the limit, at least for finite parameter spaces.

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1. Letting $\phi$ satisfy $\phi(Z) = I^Z(X; Y)$ a.s., define $I(X, Y | Z = z) = \phi(z)$. This notation is necessarily well defined only up to a null set under the marginal distribution of $Z$. 

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3
2.1 Connections between $IOMI_D(A)$ and $CMI^k_D(A)$

One of the fundamental differences between $IOMI_D(A)$ and $CMI^k_D(A)$ is that $CMI^k_D(A)$ is bounded above by $n \log k$, because $I(W; U^{(k)}|\tilde{Z}^{(k)}) \leq H(U^{(k)}) \leq n \log k$ (Steinke and Zakynthinou, 2020). In contrast, $IOMI_D(A)$ can easily become infinite even for the learning algorithms $A$ that provably generalize (Bu, S. Zou, and Veeravalli, 2019). Indeed, one of the motivations of Steinke and Zakynthinou was the fact that deterministic learning algorithms and every (possibly randomized) proper empirical risk minimization algorithm over the class of threshold functions on the real line have very large $IOMI_D(A)$ (Bassily et al., 2018). In contrast, some of these algorithms have small $CMI^k_D(A)$. In fact, $CMI^k_D(A)$ is never larger than $IOMI_D(A)$.

**Theorem 2.1.** Let $A$, $W$, $U^{(k)}$, $\tilde{Z}^{(k)}$, and $S$ be as in the introduction. Then $I(W; S) = I(W; \tilde{Z}^{(k)}) + I(W; U^{(k)}|\tilde{Z}^{(k)})$. In particular, $CMI^k_D(A) \leq IOMI_D(A)$.

**Proof.** By the chain rule for the mutual information, we have

$$I(W; U^{(k)}, \tilde{Z}^{(k)}) = I(W; \tilde{Z}^{(k)}) + I(W; U^{(k)}|\tilde{Z}^{(k)}).$$  \hspace{1cm} (1)

Since $S$ is $\sigma(\tilde{Z}^{(k)}, U^{(k)})$-measurable, $I(W; U^{(k)}, \tilde{Z}^{(k)}) = I(W; S, U^{(k)}, \tilde{Z}^{(k)})$. But then $W$ is independent of $\tilde{Z}^{(k)}, U^{(k)}$ given $S$, hence $I(W; S, U^{(k)}, \tilde{Z}^{(k)}) = I(W; S)$. The result follows from the nonnegativity of mutual information.

In the next theorem, we demonstrate that taking $k$ to infinity in Definition 1.2, the $CMI^k_D(A)$ recovers the $IOMI_D(A)$ for the case when the parameter space is finite.

**Theorem 2.2.** Assume the output of $A$ takes value in a finite set. Then

$$\lim_{k \to \infty} CMI^k_D(A) = IOMI_D(A).$$

**Proof.** By Theorem 2.1, $I(W; U^{(k)}|\tilde{Z}^{(k)}) = I(W; S) - I(W; \tilde{Z}^{(k)})$. Therefore, in order to prove the claim, we need to show $\lim_{k \to \infty} I(W; \tilde{Z}^{(k)}) = 0$ when $I(W; S)$ is finite.

Recall that $A$ is a probability kernel from the space of tuples in $\mathcal{Z}$ to $\mathcal{W}$. Assume $\mathcal{W} = \{w_1, \ldots, w_m\}$. For each $i \in [m]$, let $\kappa_i(S) = \mathbb{P}[W = w_i]$ and $f_i : \mathcal{Z}^{kn} \to [0, 1]$ be a measurable function defined as

$$f_i(\tilde{Z}^{(k)}) = \frac{1}{k^n} \sum_{w \in [k]^n} \kappa_i(\tilde{Z}^{(k)}_w).$$

Letting $z, z' \in \mathcal{Z}^{kn}$ be two super-samples that only differ in one element, it is straightforward to see that

$$|f_i(z) - f_i(z')| \leq \frac{1}{k}.$$

Therefore, we can invoke McDiarmid’s inequality to obtain

$$\mathbb{P}[|f_i(\tilde{Z}^{(k)}) - \mathbb{E}[f_i(\tilde{Z}^{(k)})]| \geq \varepsilon] \leq \exp\left(-\frac{2k\varepsilon^2}{n}\right).$$  \hspace{1cm} (2)

Also, we have $\mathbb{E}[f_i(\tilde{Z}^{(k)})] = \mathbb{P}[W = w_i]$ as each element of $\tilde{Z}^{(k)}$ is IID. Hence, $f_i(\tilde{Z}^{(k)}) \to \mathbb{P}[W = w_i]$ in probability as $k$ diverges.
By the definition of mutual information and KL divergence,

\[
I(W; Z^{(k)}) = \mathbb{E}[\text{KL}(\mathbb{P}^{(k)}[W] \| \mathbb{P}[W])]
\]

\[
= \mathbb{E}\left[\text{KL}\left(\frac{1}{k^n} \sum_{u} \mathbb{P}^{(k)}_{Z_u}[W] \| \mathbb{P}[W]\right)\right]
\]

\[
= \sum_{l} \mathbb{E}\left[\frac{1}{k^n} \sum_{u} \kappa_l(\tilde{Z}^{(k)}_u) \log \frac{\mathbb{P}[W = w_l]}{\mathbb{P}[W]}\right]
\]

\[
= \sum_{l} \mathbb{E}\left[f_l(\tilde{Z}^{(k)}) \log \frac{\mathbb{P}[W = w_l]}{\mathbb{P}[W]}\right]. \quad (3)
\]

Defining \(\phi_l : [0,1] \to \mathbb{R}\) as \(\phi_l(x) = x \log \frac{x}{\mathbb{P}[W = w_l]}\), we have established

\[
I(W; Z^{(k)}) = \sum_{l} \mathbb{E}\left[\phi_l(\tilde{Z}^{(k)})\right]. \quad (4)
\]

Note that \(\phi_l\) is a continuous and bounded function. By a standard result (Durrett, 2019, Thm. 2.3.4), \(f_l(\tilde{Z}^{(k)}) \to \mathbb{P}[W = w_l]\) in probability implies that

\[
\mathbb{E}\left[\phi_l(\tilde{Z}^{(k)})\right] \to \mathbb{E}\left[\phi_l(\mathbb{P}[W = w_l])\right] = 0,
\]

as \(k\) goes to infinity. Using this, we conclude that \(I(W; Z^{(k)}) \to 0\) as \(k\) diverges, as was to be shown.

\[\square\]

3 Sharpened Bounds based on Individual Samples

In this section, we present two novel generalization bounds and show that they provide a tighter characterization of the generalization error compared to Theorem 1.3 by Steinke and Zakynthinou (2020). The results are inspired by the improvements on IOMI\(_D\)(\(\mathcal{A}\)) made by Bu, S. Zou, and Veeravalli (2019). In particular, Theorem 3.1 bounds the expected generalization error in terms of the mutual information between the output parameter and a random subsequence of the indices \(U\), given the super-sample. Then, in Theorem 3.4, we derive a generalization bound that is constructed in terms of the (disintegrated) mutual information between each individual element of \(U\) and the output of the learning algorithm, \(W\). The bound in Theorem 3.4 is an analogue of (Bu, S. Zou, and Veeravalli, 2019, Prop. 1) for Theorem 1.3.

For the remainder of this section, let \(\mathcal{A}, W, U^{(k)}, Z^{(k)}\), and \(S\) be as in the introduction with \(k = 2\). To ease notational burden, we will drop the superscript from \(U^{(k)}\) when the value of \(k\) is clear from context. Let \(U = (U_1, \ldots, U_n)\).

**Theorem 3.1.** Fix \(m \in [n]\) and let \(J = (J_1, \ldots, J_m)\) be a random subset of \([n]\), distributed uniformly among all subsets of size \(m\) and independent from \(W, Z^{(2)}, \) and \(U\). Then

\[
\text{EGE}_D(\mathcal{A}) \leq \mathbb{E} \sqrt{\frac{2}{m} \mathbb{E}[Z^{(2)}(W; U_J) | J].} \quad (5)
\]

**Proof.** With \(k = 2\), recall from the introduction

\[
Z^{(2)} = \begin{pmatrix} Z_{1,1} & \cdots & Z_{1,n} \\ Z_{2,1} & \cdots & Z_{2,n} \end{pmatrix} \sim \mathcal{D}^{2n},
\]

and \(U = (U_1, \ldots, U_n) \in \{1,2\}^n\) where \(U_i\)s are IID, and the marginal distribution follows \(U_i \sim \text{Bern}\left(\frac{1}{2}\right)\) for \(i \in [n]\). Furthermore, recall \(S = \{Z_{U_{i,1}}, \ldots, Z_{U_{i,n}}\}\). The expected gen-
eralization error can be written as
\[
\mathbb{E} \left[ R_D(W) - R_S(W) \right] = \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} (-1)^{U_i} (\ell(Z_{1,i},W) - \ell(Z_{2,i},W)) \right]
\]
where the last equality follows because \( J \) is independent of \( U_j, Z^{(2)} \) and \( W \).

Define \( W, U_j, \) and \( J \) such that \((W, U_j, J, Z^{(2)}) \) \( \equiv (W, U_j, Z^{(2)}) \), and \( \hat{W}, U_j, \) and \( J \) are independent given \( Z^{(2)} \). By the Donsker–Varadhan variational formula (Boucheron, Lugosi, and Massart, 2013, Prop. 4.15) and the disintegration theorem (Kallenberg, 2006, Thm. 6.4), for all measurable functions \( g \) in \( G \), i.e., the class of all functions \( g \) such that \( \mathbb{P}^2(\hat{W} \otimes \mathbb{P}^2(U_j) \otimes \mathbb{P}^2(J)) (\exp g) < \infty \), with probability one we have
\[
I^{(2)}(W, J; U_j) = \text{KL}(\mathbb{P}^2[W, J, U_j] \| \mathbb{P}^2(W) \otimes \mathbb{P}^2(J) \otimes \mathbb{P}^2(U_j))
\]
\[
= \sup_{g \in G} \mathbb{P}^2(W, J, U_j)(g) - \log \left( \mathbb{P}^2(\hat{W} \otimes \mathbb{P}^2(U_j) \otimes \mathbb{P}^2(J)) (\exp g) \right).
\]
Define \( f(w, j, u_j) \triangleq \frac{\lambda}{m} \sum_{i=1}^{m} (-1)^{U_i} (\ell(z_{1,i}, w) - \ell(z_{2,i}, w)) \) where \( \lambda \geq 0 \). By Eq. (9), we can write
\[
I^{(2)}(W, J; U_j) \geq \mathbb{P}^2(W, U_j, J)(f) - \log \left( \mathbb{P}^2(\hat{W} \otimes \mathbb{P}^2(U_j) \otimes \mathbb{P}^2(J)) (\exp f) \right).
\]

Considering the second term of the RHS of Eq. (10), Hoeffding’s lemma implies that
\[
\left( \mathbb{P}^2(\hat{W} \otimes \mathbb{P}^2(U_j) \otimes \mathbb{P}^2(J)) (\exp f) \right)
\]
\[
= \mathbb{E}^{(2)} \exp \left( \frac{\lambda}{m} \sum_{i=1}^{m} (-1)^{U_i} \left( \ell(Z_{1,i}, \hat{W}) - \ell(Z_{2,i}, \hat{W}) \right) \right)
\]
\[
= \mathbb{E}^{(2)} \mathbb{E}^{(2)}[\hat{W}] \prod_{i=1}^{m} \exp \left( \frac{\lambda}{m} (-1)^{U_i} \left( \ell(Z_{1,i}, \hat{W}) - \ell(Z_{2,i}, \hat{W}) \right) \right)
\]
\[
\leq \mathbb{E}^{(2)} \mathbb{E}^{(2)}[\hat{W}] \prod_{i=1}^{m} \exp \left( \frac{\lambda^2}{2m^2} \left( \ell(Z_{1,i}, \hat{W}) - \ell(Z_{2,i}, \hat{W}) \right)^2 \right)
\]
\[
\leq \exp \left( \frac{\lambda^2}{2m} \right),
\]
where we use the fact that \( \left( \mathbb{P}^2(\hat{W} \otimes \mathbb{P}^2(U_j) \otimes \mathbb{P}^2(J)) (f) \right) = 0 \).

Substituting the bound in Eq. (15) into Eq. (10), rearranging and taking expectations, we obtain
\[
\mathbb{E} \left[ \frac{1}{m} \sum_{i=1}^{m} (-1)^{U_i} (\ell(Z_{1,i}, W) - \ell(Z_{2,i}, W)) \right] \leq \mathbb{E} \inf_{\lambda \geq 0} \frac{I^{(2)}(W, J; U_j) + \frac{\lambda^2}{2m}}{\lambda}
\]
\[
= \mathbb{E} \sqrt{\frac{2}{m} I^{(2)}(W, J; U_j)}.
\]
Moreover, we have a.s.
\[
I^{(2)}(J, W; U_j) - \sqrt{\frac{2}{m} I^{(2)}(J; U_j)} = I^{(2)}(W; U_j | J).
\]
Here, $I^{(2)}(J; U_J) = 0$ since $J$ is independent of $U_J$ given $\tilde{Z}^{(2)}$. Plugging Eq. (18) into Eq. (17), we obtain the desired result. \hfill \Box

In the next theorem, we show that the generalization bound in Theorem 3.1 is tighter than the bound in Theorem 1.3 by Steinke and Zakynthinou (2020).

**Theorem 3.2.** Let $m_1, m_2 \in [n]$ such that $1 \leq m_1 < m_2 \leq n$, and let $J^{(m_1)}, J^{(m_2)}$ be random subsets of $[n]$, distributed uniformly among all subsets of size $m_1$ and $m_2$, respectively, and independent from $W, \tilde{Z}^{(2)},$ and $U$. Then

$$
\frac{1}{m_1} I(W; U_{j^{(m_1)}} | \tilde{Z}^{(2)}, J^{(m_1)}) \leq \frac{1}{m_2} I(W; U_{j^{(m_2)}} | \tilde{Z}^{(2)}, J^{(m_2)}).
$$

(19)

In particular,

$$
\mathbb{E} \sqrt{\frac{2}{m} J^{(2)}(W; U_J) \leq \sqrt{\frac{2}{m} I(W; U | \tilde{Z}^{(2)})}.}
$$

(20)

**Proof.** Consider

$$
I(W; U_{j^{(m_1)}} | \tilde{Z}^{(2)}, J^{(m_1)}) = H(U_{j^{(m_1)}} | \tilde{Z}^{(2)}, W) - H(U_{j^{(m_1)}} | \tilde{Z}^{(2)})
$$

(21)

$$
= \frac{1}{(m_1)} \sum_{K_1 \in [n] \setminus m_1} H(U_{K_1} | \tilde{Z}^{(2)}) - H(U_{j^{(m_1)}} | \tilde{Z}^{(2)}, W)
$$

(22)

$$
= \frac{1}{(m_1)} \sum_{K_1 \in [n] \setminus m_1} H(U_{K_1} | \tilde{Z}^{(2)}) - \frac{1}{(m_1)} \sum_{K_1 \in [n] \setminus m_1} H(U_{K_1} | \tilde{Z}^{(2)}, W)
$$

(23)

Eq. (22) follows because $\tilde{Z}^{(2)} \perp \tilde{J}^{(m_1)}$, while Eq. (23) follows because the event $\{j^{(m_1)} = K_1\}$ is independent of $(W, U_{K_1}, \tilde{Z}^{(2)})$. Then

$$
\frac{1}{m_1} I(W; U_{j^{(m_1)}} | \tilde{Z}^{(2)}, J^{(m_1)}) = \frac{1}{m_1} \sum_{K_1 \in [n] \setminus m_1} [H(U_{K_1}) - H(U_{K_1} | \tilde{Z}^{(2)})]
$$

(24)

$$
= \frac{1}{m_1} [H(U) - \frac{1}{m_1} \sum_{K_1 \in [n] \setminus m_1} H(U_{K_1} | \tilde{Z}^{(2)})]
$$

(25)

$$
= \frac{1}{m_2} \sum_{K_2 \in [n] \setminus m_2} H(U_{K_2}) - \frac{1}{m_1} \sum_{K_1 \in [n] \setminus m_1} H(U_{K_1} | \tilde{Z}^{(2)})
$$

(26)

$$
\leq \frac{1}{m_2} \sum_{K_2 \in [n] \setminus m_2} [H(U_{K_2}) - H(U_{K_2} | \tilde{Z}^{(2)})]
$$

(27)

$$
= \frac{1}{m_2} I(W; U_{j^{(m_2)}} | \tilde{Z}^{(2)}, J^{(m_2)}).
$$

(28)

Eq. (24) follows from Eq. (23) and the fact that $U \perp \tilde{Z}^{(2)}$, while Eq. (25) follows from each element of $U$ being IID. Eq. (27) follows from Lemma C.1, which is a modified version of the Han’s inequality (Te Sun, 1978). Finally, the last step follows from using the same line of reasoning as in Eq. (21) to Eq. (23).

Having established Eq. (19), the claim follows from

$$
\mathbb{E} \sqrt{\frac{2}{m} J^{(2)}(W; U_J) \leq \sqrt{\frac{2}{m} I(W; U | \tilde{Z}^{(2)})}
$$

(29)

$$
\leq \sqrt{\frac{2}{m} I(W; U | \tilde{Z}^{(2)})}
$$

(30)

where Eq. (29) is Jensen’s inequality, and Eq. (30) is the direct application of Eq. (19) with $m_1 = m$ and $m_2 = n$. This proves the desired result. \hfill \Box
Applying Jensen’s inequality to Theorem 3.1, we obtain

$$\mathbb{E} \left[ R_D(W) - \hat{R}_S(W) \right] \leq \sqrt{\frac{2}{m} I(W; U_j | Z^{(2)}, J)}.$$  \hspace{1cm} (31)

Then, an application of the result in Eq. (19) lets us compare the bound in Eq. (31) for different values of the cardinality $J$. We summarize this result in the next corollary.

**Corollary 3.3.** We have

$$\mathbb{E} G E_D(A) \leq \sqrt{\frac{2}{m} I(W; U_j | Z^{(2)}, J)},$$  \hspace{1cm} (32)

where the case $m = \# J = n$ is equivalent to Theorem 1.3. Further, the bound is increasing with respect to $m$ for $m \in [n]$. In particular, the tightest bound is achieved when $m = \# J = 1$.

Our next result shows that that we can pull the expectation over both $Z^{(2)}$ and $J$ outside the concave square-root function.

**Theorem 3.4.** Let $J$ be a uniformly distributed element in $[n]$, independent from $W, Z^{(2)}$, and $U$. Then

$$\mathbb{E} G E_D(A) \leq \mathbb{E} \sqrt{2I^{(2)}(W; U_j)} = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \sqrt{2I^{(2)}(W; U_i)}. \hspace{1cm} (33)$$

**Proof.** By the Donsker–Varadhan variational formula (Boucheron, Lugosi, and Massart, 2013, Prop. 4.15) and the disintegration theorem (Kallenberg, 2006, Thm. 6.4), with probability one, for all measurable functions $g$ such that $(\mathbb{P}^{Z^{(2)}}[\tilde{W}] \otimes \mathbb{P}^{Z^{(2)}}[\tilde{U}_i])(\exp g) < \infty$, we have

$$I^{(2)}(U_i, W) = KL(\mathbb{P}^{Z^{(2)}}[U_i, W] \| \mathbb{P}^{Z^{(2)}}[\tilde{U}_i] \otimes \mathbb{P}^{Z^{(2)}}[\tilde{W}]) \geq \mathbb{P}^{Z^{(2)}}[U_i, W][g(W, Z^{(2)}, U_i)] - \log \mathbb{P}^{Z^{(2)}}[\tilde{U}_i] \otimes \mathbb{P}^{Z^{(2)}}[\tilde{W}][\exp(g(\tilde{W}, \tilde{Z}^{(2)}, \tilde{U}_i))].$$  \hspace{1cm} (34)

where $(W, U_i, Z^{(2)}) \overset{d}{=} (\tilde{W}, \tilde{U}_i, \tilde{Z}^{(2)})$ and $W \perp \perp \tilde{U}_i | \tilde{Z}^{(2)}$. For $i \in [n]$, let

$$g_i(W, Z^{(2)}, U_i) \triangleq \lambda (-1)^{U_i}(\ell(Z_{1,i}, W) - \ell(Z_{2,i}, W)).$$

Hoeffding’s lemma implies that

$$\mathbb{P}^{Z^{(2)}}[\tilde{U}_i] \otimes \mathbb{P}^{Z^{(2)}}[\tilde{W}][\exp(g_i(\tilde{W}, \tilde{Z}^{(2)}, \tilde{U}_i))] \leq \exp \left( \frac{\lambda^2}{2} \right),$$  \hspace{1cm} (35)

where in the last line we have used $g_i \in [-\lambda, \lambda]$ a.s. From (35), we obtain

$$\mathbb{E}^{Z^{(2)}} \left( -1 \right)^{U_i}(\ell(Z_{1,i}, W) - \ell(Z_{2,i}, W)) \leq \inf_{\lambda \geq 0} \frac{KL(\mathbb{P}^{Z^{(2)}}[U_i, W] \| \mathbb{P}^{Z^{(2)}}[\tilde{U}_i] \otimes \mathbb{P}^{Z^{(2)}}[\tilde{W}]) + \frac{\lambda^2}{2}}{\lambda}.$$  \hspace{1cm} (36)

Then, averaging over $i$ and taking expectations,

$$\mathbb{E} \left[ R_D(W) - \hat{R}_S(W) \right] = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}^{Z^{(2)}} \left( -1 \right)^{U_i}(\ell(Z_{1,i}, W) - \ell(Z_{2,i}, W)) \leq \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \sqrt{2I^{(2)}(W; U_i)}. \hspace{1cm} (37)$$

$$= \sqrt{2I^{(2)}(W; U_i)}.$$  \hspace{1cm} (38)
Remark 3.5. We can show that the bound in Theorem 3.4 provides a tighter characterization of the expected generalization error than Theorem 1.3 by Steinke and Zakynthinou (2020). To show this, we can write
\[ \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}[\sqrt{2I(\tilde{Z}(2); U_i)}] \leq \sqrt{\frac{2}{n} I(Z; U_1|\tilde{Z}(2))} \]
(41)
Here, the first inequality follows from Jensen’s inequality, while the second follows from the independence of indices \( U_i \).

Remark 3.6. For the case where \( |J| = 1 \), the bound in Theorem 3.4 is tighter than the bound in Theorem 3.2 because the expectation with respect to \( J \) happens outside of the strictly concave square-root function.

4 Generalization bounds for noisy, iterative algorithms

In this section, we investigate this new class of generalization bounds in the context of nonconvex learning. In particular, we analyze Langevin dynamics (LD) algorithm (Gelfand and Mitter, 1991), following the analysis pioneered by Pensia, Jog, and Loh (2018). Our approach is similar to the recent advances by Negrea et al. (2019) and Li, Luo, and Qiao (2020), who employ data-dependent estimates to obtain bounds that are easily estimated. We will see that the use of the generalization bound in Section 3 allows us to exploit past iterates to tighten the bounds. The influence of past iterates are seen to take the form of a hypothesis test.

4.1 Bounding Generalization Error via Hypothesis Testing

First, we present the following well-known result that allows one to bound mutual information by the expectation of the KL divergence of a conditional distribution (“posterior”) with respect to a “prior”. The statement of the following lemma is taken from Negrea et al. (2019).

Lemma 4.1. Let \( X \) and \( Y \) be random elements. Then, for all probability measures \( P \) on the same space as \( Y \), \( I(X; Y) \leq \mathbb{E}[\text{KL}(P^X[Y] \| P)] \), with equality for \( P = \mathbb{E}[P^X[Y]] = P[Y] \). Moreover, given another random element \( Z \), it follows immediately by the disintegration theorem (Kallenberg, 2006, Thm. 6.4) that, for all \( Z \)-measurable random probability measures \( P \) on the same space as \( Y \),
\[ I(Z; X|Y) \leq \mathbb{E}_Z[\text{KL}(P^X[Y] \| P)] \text{ a.s.,} \]
with a.s. equality for \( P = \mathbb{E}_Z[P^X[Y]] = P_Z[Y] \).

In our setting, the “posterior” of \( W \) given \( S \), which is denoted \( Q \), is the conditional distribution of \( W \) given \( S \).

We begin by combining Lemma 4.1 with Theorem 1.3 to obtain
\[ \mathbb{E}[\text{GE}_D(A)] \leq \sqrt{\frac{2}{n} I(Z; U|\tilde{Z}(2))} \leq \sqrt{\frac{2}{n} \mathbb{E}[\text{KL}(Q \| P(\tilde{Z}(2)))]} \]
(42)
Here we have used \( \mathbb{P}_Z(\tilde{Z}|W) = \mathbb{P}_S[W] = Q \text{ a.s.} \) Note that the prior, i.e., \( P \) in Eq. (42) has only access to \( \tilde{Z}(2) \), therefore the training set can take \( 2^n \) different values. Next, we demonstrate that our generalization bound in Theorem 3.1 can be upper bounded using \( \text{KL}(Q \| P) \),
where the prior $P$ has access to the information in the training set, i.e., $S$. Another application of Lemma 4.1 to the bound in Theorem 3.1 yields

$$\text{EGE}_{D}(A) \leq E \sqrt{\frac{2}{m} \mathbb{E} Z^{(2)}(W; U_j | U_F, J)}$$
$$\leq E \sqrt{\frac{2}{m} \mathbb{E} Z^{(2)}[\text{KL}(Q \| P(Z^{(2)}, U_F, J))]}. \quad (43)$$

Here the bound in Eq. (43) contains a prior that has access to $n - m$ samples in the training set, i.e., $S_F$, because $\tilde{Z}^{(2)}_{U_j} = S_F$. The rest of the training set, $S_j$, is unknown to $P$. However, since $\tilde{Z}^{(2)}$ is known to the prior, the training set can take finitely many distinct values, i.e., $2^m$. Comparing Eq. (42) to Eq. (43) we see that a data-dependent prior reduces the number of distinct values that the training set $S$ takes from $2^n$ to $2^m$. It is important to note that the bound in Eq. (43) is loser than the bound we started with in Theorem 3.1 as conditioning increases the mutual information. Nevertheless, the KL divergence based on $P$ can exploit the information in the training set to obtain tighter bounds on the mutual information.

Next, we formally state the chain rule for KL divergence that is the main ingredient of our method to obtain generalization error bounds for iterative algorithms. We start by setting some notation. For $T \in \mathbb{N}$, let $[T]_0 = \{0, 1, 2, \ldots, T\}$. Let $v$ denote a distribution on $W^{[T]_0}$, and $X$ be a random variable with distribution $v$. For $t \in [T]_0$, we will use the following notations for certain conditional and marginal distributions:

i) $v_t = P[X_t]$, the marginal law of $X_t$;
ii) $v_{t-1} = P[X_{t-1} | X_t]$, the conditional law of $X_t$ given $X_{t-1}$; and
iii) $v_{0:t} = P[X_{0:t}]$, the marginal law of $X_{0:t}$.

**Lemma 4.2 (Chain Rule for KL Divergence).** Let $Q, P$ be probability measures on $W^{[T]_0}$. Suppose that $Q_0 = R_0$. Then

$$\text{KL}(Q_T \| P_T) \leq \text{KL}(Q \| P) = \sum_{t=1}^{T} E_{Q_{0:t-1}}[\text{KL}(Q_t \| P_t)].$$

where, $Q_t$ is the conditional law of $t$-th iterate given the previous iterates, and so $\text{KL}(Q_t \| P_t)$ is a random variable which depends the $(W_0, \ldots, W_{t-1}) \sim Q_{0:t-1}$.

The chain rule (Lemma 4.2) allows us to bound the KL divergence involving the terminal parameter with one involving the sum of the KL divergence over each individual step for the full trajectory. The benefit of using chain rule for analyzing the iterative algorithm are two fold. First, we gain analytical tractability when analyzing iterative learning algorithms stepwise. In fact, many bounds that appear in the literature implicitly require this form of incrementation (Pensia, Jog, and Loh, 2018; Bu, S. Zou, and Veeravalli, 2019; Negrea et al., 2019; Li, Luo, and Qiao, 2020). Second, the information in the optimization trajectory can be exploited to identify which parameter $U$ generates $W$. Specifically, consider the generalization bound in Eq. (43) and the chain rule for KL in Lemma 4.2. Then, we have

$$\text{KL}(Q_T \| P_T(\tilde{Z}^{(2)}, U_F, J)) \leq \sum_{t=1}^{T} E_{Z^{(2)}, U_F, J}[\text{KL}(Q_t \| P_t)].$$

Here $P_t$ is a $\sigma(\tilde{Z}^{(2)}, U_F, J, W_{0:t-1})$-measurable random probability measure. The prior may use $U_F$, $\tilde{Z}^{(2)}$, and $J$ to reduce the number of possible values that $U$ can take to $2^{|J|}$. Moreover, since during optimization, $U_j$ is the same, $W_0, W_1, W_2, \ldots, W_{t-1}$ may leak some information about $U_j$, and the prior could use this information to tighten the bound by choosing a $P_t$ which achieves small KL$(Q_t \| P_t)$. For instance, provided that using $W_0, W_1, W_2, \ldots, W_{t-1}$ the prior can perfectly estimate $U_j$, then we can set $P_t = Q_t$ and KL$(Q_t \| P_t)$ will be zero. As will be seen in the text subsection, we explicitly design a prior that use the information in the optimization trajectory for LD algorithm. Nevertheless, considering the KL between full trajectories may yield a loose upper bound on the KL between terminal parameters.
4.1.1 Tighter Generalization bound for the case \( m = 1 \)

In the next theorem, for the case with \( m = 1 \), we provide a tighter bound compared to Eq. (43) by showing that one can pull the expectation over both \( U_{Ic} \) and \( J \) outside the concave square-root function. Note that it is incomparable for other values of \( m \).

**Theorem 4.3.** Let \( W, U \triangleq (U_1, \ldots, U_n), Z^{(k)}, \) and \( S \) be as in the introduction with \( k = 2 \). Let \( J \) be a random index in \([n]\) sampled uniformly at random without replacement with a sampling procedure which is independent from \( W, U, \) and \( Z^{(2)} \). Let \( Q \subseteq \mathbb{P}Z^{(2)}UW \) and \( P \) be a \( \sigma(Z^{(2)}, U_{Ic}, J) \)-measurable random probability measure. Then

\[
\mathbb{E} \left[ \mathcal{D}(A) \right] \leq \mathbb{E} \sqrt{2 \text{KL}(Q||P)}.
\]

The proof is deferred to Appendix B. Note that the KL divergence is between two random measures and, hence, is a random variable. In particular, it is \( \sigma(Z^{(2)}, J, U) \)-measurable, and so the expectation averages over these variables.

4.2 Example: Langevin Dynamics Algorithm

In this subsection we give generalization bounds for gradient-based iterative noisy algorithms. In particular, we focus on the LD algorithm. In the setting of classification and continuous parameter spaces, the empirical risk function does not provide useful gradients. In this case, it is common to optimize a surrogate objective, constructed from a surrogate loss, such as cross entropy. Write \( \ell : \mathcal{Z} \times \mathcal{W} \rightarrow \mathbb{R} \) for the surrogate loss and let \( \tilde{R}_S(w) = \frac{1}{n} \sum_{i=1}^n \tilde{\ell}(Z_i, w) \) be the empirical surrogate risk.

Let \( \eta_t \) be the learning rate at time \( t \), \( \beta_t \) the inverse temperature at time \( t \) and let \( \epsilon_i \) be sampled i.i.d. from \( \mathcal{N}(0, I_d) \). LD algorithm iterates are given by

\[
W_{t+1} = W_t - \eta_t \nabla \tilde{R}_S(W_t) + \sqrt{2 \eta_t/\beta_t} \epsilon_i,
\]

where \( \tilde{R}_S(w) = \frac{1}{n} \sum_{z \in S} \tilde{\ell}(w, z) \).

**Theorem 4.4 (Generalization bound for LD algorithm).** Let \( \{W_t\}_{t \in [T]} \) denote the iterates of the LD algorithm. If \( \ell(Z, W) \) is \([0, 1]\)-bounded then

\[
\mathbb{E} \left[ R_D(W_T) - \tilde{R}_S(W_T) \right] \leq \frac{1}{n\sqrt{2}} \inf_{\theta \in \Theta} \mathbb{E} \left[ \sum_{t=0}^{T-1} \mathbb{E} \left[ Z_{1:J}^{(2)}, U, J \right] \beta_t \eta_t \|\zeta_t\|^2 \left( \mathbb{I} \{U_J = 1\} - \theta \left( \sum_{i=0}^{T-1} (Y_{t,2} - Y_{t,1}) \right) \right)^2 \right].
\]  

Here, we define two-sample incoherence at time \( t \)

\[
\zeta_t = \nabla \tilde{\ell}(Z_{1:J}, W_t) - \nabla \tilde{\ell}(Z_{2:J}, W_t).
\]

\( \Theta \) denotes the family of measurable functions such that for any \( \theta \in \Theta \) we have \( \theta : \mathbb{R} \rightarrow [0, 1] \). Also, for \( t \geq 1 \), \( Y_{t,1} \) and \( Y_{t,2} \) are given by

\[
Y_{t,1} \triangleq \sum_{i=1}^{t} \frac{\beta_{i-1}}{4\eta_{i-1}} \|W_i - W_{i-1} + \eta_{i-1} \alpha_n - \nabla \tilde{R}_S(W_{i-1}) + \frac{\eta_{i-1}}{n} \nabla \tilde{\ell}(Z_{1:J}, W_{i-1}) \|^2,
\]

\[
= \mathbb{I} \{U_J = 1\} \sum_{i=1}^{t} \left( \|\epsilon_i\|^2 + \mathbb{I} \{U_J = 2\} \sum_{i=1}^{t} \frac{1}{2} \|\zeta_i + \epsilon_i\|^2 \right),
\]

and

\[
Y_{t,2} \triangleq \sum_{i=1}^{t} \frac{\beta_{i-1}}{4\eta_{i-1}} \|W_i - W_{i-1} + \eta_{i-1} \alpha_n - \nabla \tilde{R}_S(W_{i-1}) + \frac{\eta_{i-1}}{n} \nabla \tilde{\ell}(Z_{2:J}, W_{i-1}) \|^2,
\]

\[
= \mathbb{I} \{U_J = 1\} \sum_{i=1}^{t} \left( \|\epsilon_i\|^2 + \frac{\sqrt{\beta_{i-1}\eta_{i-1}}}{n\sqrt{2}} \|\zeta_i + \epsilon_i\|^2 \right) + \mathbb{I} \{U_J = 2\} \sum_{i=1}^{t} \frac{1}{2} \|\epsilon_i\|^2,
\]

where \( Y_{0,1} = Y_{0,2} = 0 \).
In the next remark, we provide a simplification of the bound in Eq. (46).

**Remark 4.5.** Consider \( \theta \in \Theta \) that satisfies the property \( 1 - \theta(x) = \theta(-x) \). Then, we can simplify Eq. (46) to

\[
\mathbb{E} \left[ R_D(W_T) - \hat{R}_S(W_T) \right] \leq \frac{1}{n\sqrt{2}} \sqrt{n \sum_{t=0}^{T-1} \mathbb{E} \left[ \mathbb{E}^{(2)}(U_t, J_t = q) \beta_t \eta_t \| \xi_t \|^2 \left( 1 \{ q = 1 \} - \theta \left( \sum_{i=0}^{t} (Y_t, Y_{t+1}) \right) \right)^2 \right].
\]

For instance, \( \theta(x) = \frac{1}{2} + \frac{1}{2} \tanh(x) \) and \( \hat{\theta}(x) = \frac{1}{2} + \frac{1}{2} \text{erf}(x) \) satisfy \( 1 - \theta(x) = \theta(-x) \).

In the next remark, we discuss the number of samples required to estimate the generalization bound in Theorem 4.4.

**Remark 4.6.** By the law of total expectation, for any \( \theta \in \Theta \) we can write

\[
\mathbb{E} \left[ R_D(W_T) - \hat{R}_S(W_T) \right] \leq \frac{1}{2 \sqrt{2n}} \mathbb{E} [T_1 + T_2],
\]

where

\[
T_q \triangleq \frac{1}{n \sqrt{2}} \sqrt{n \sum_{t=0}^{T-1} \mathbb{E} \left[ \mathbb{E}^{(2)}(U_t, J_t = q) \beta_t \eta_t \| \xi_t \|^2 \left( 1 \{ q = 1 \} - \theta \left( \sum_{i=0}^{t} (Y_t, Y_{t+1}) \right) \right)^2 \right].
\]

for \( q \in \{1, 2\} \). Here \( T_1 \) and \( T_2 \) can be estimated from \( n + 1 \) points \( \{Z_1, \ldots, Z_{J-1}, Z_{J+1}, \ldots, Z_n\} \cup \{Z_t, Z_{t+1}\} \sim D^{n+1} \). In particular to estimate \( T_1 \) for a fixed \( J \), the training set is \( S_1 = \{Z_1, \ldots, Z_J, Z_{J+1}, \ldots, Z_n\} \). Similarly \( T_2 \), can be estimated when the training set is \( S_2 = \{Z_1, \ldots, Z_{J+1}, Z_{J+2}, \ldots, Z_n\} \). Ergo, to estimate the inner expectation we need only \( n + 1 \) points.

The generalization bound in Eq. (46) does not place any restrictions on the learning rate or Lipschitz continuity of the loss or its gradient. In the next corollary we study the asymptotic properties of the bound in Eq. (46) when \( \tilde{\ell} \) is \( L \)-Lipschitz. Then, we draw a comparison between the bound in this paper and some of the existing bounds in the literature.

**Corollary 4.7.** Under the assumption that \( \tilde{\ell} \) is \( L \)-Lipschitz, we have \( \| \xi_t \| \leq 2L \). Then, the generalization bound in Eq. (46) can be upper-bounded as

\[
\mathbb{E} (R_D(W_T) - R_S(W_T)) \leq \frac{\sqrt{2L}}{n} \inf_{\theta \in \Theta} \frac{1}{n \sqrt{2}} \sqrt{n \sum_{t=0}^{T-1} \mathbb{E} \left[ \mathbb{E}^{(2)}(U_t, J_t = q) \beta_t \eta_t \left( 1 \{ q = 1 \} - \theta \left( \sum_{i=0}^{t} (Y_t, Y_{t+1}) \right) \right)^2 \right]}. \]

**Remark 4.8.** Li, Luo, and Qiao (2020, Thm. 9) have the following bound for LD algorithm under the \( L \)-Lipschitz assumption.

\[
\mathbb{E} [R_D(W_T) - R_S(W_T)] \leq \frac{\sqrt{2L}}{n} \sqrt{\sum_{t=0}^{T-1} \beta_t \eta_t}. \]

We can immediately see that Eq. (52) can provide tighter upper bound compared to Eq. (53) by setting \( \theta(x) = \frac{1}{2}, \forall x \in \mathbb{R} \). Also, our bound has order-wise improvement with respect to \( n \) over the bounds in Bu, S. Zou, and Veeravalli (2019) and Pensia, Jog, and Loh (2018) under the \( L \)-Lipschitz assumption. Negrea et al. (2019, App. E.1) obtain a bound

\[
\mathbb{E} [R_D(W_T) - R_S(W_T)] \leq \frac{L}{2(n-1)} \sqrt{\sum_{t=0}^{T-1} \beta_t \eta_t}. \]
It is unclear without further context to compare the bound in Eq. (54) with the generalization bound in Eq. (52). Also, it should be noted that in contrast to (Pensia, Jog, and Loh, 2018; Bu, S. Zou, and Veeravalli, 2019; Negrea et al., 2019; Li, Luo, and Qiao, 2020) by choosing a non-constant $\theta$, our generalization bound in fact exploits the optimization trajectory as well as data to tighten the generalization bound.

\textbf{Proof of Theorem 4.4.} Considering the generalization bound in Theorem 4.3 and Lemma 4.1, we can write

$$E \left[ R_D(W) - \hat{R}_S(W) \right] \leq E \sqrt{2KL(Q_T(S) \parallel P_T(\hat{Z}^2, U_J, J))} \leq E \left[ \sum_{t=1}^{T} 2E_{Z(s), U_J} KL(Q_{\parallel P_i}) \right].$$

\hspace{1cm} (55)

First, note that from Eq. (45) it follows that

$$Q_i = N(\mu_{Q_i}, \frac{2\eta_{\parallel d}}{\beta_i}),$$

where the mean is given by

$$\mu_{Q_i} = W_{i-1} - \eta_{i-1} \frac{n-1}{n} \nabla \hat{R}_{S_i} (W_{i-1}) - \eta_{i-1} \frac{n}{n} \left( \mathbb{I} \{U_J = 1\} \nabla \ell(Z_{1, J}, W_{i-1}) + \mathbb{I} \{U_J = 2\} \nabla \ell(Z_{2, J}, W_{i-1}) \right).$$

Next, we propose the following construction of $P_i$. Note that $P_i$ is $\mathcal{F}_t$-measurable random probability measure where

$$\mathcal{F}_t = \sigma(S, Z, J, W_{i-1}).$$

Hence we can exploit the information in the trajectory up to time $t$ to construct $P_i$. In particular, we use the information in $\mathcal{F}_t$ to perform a binary hypothesis testing in which the two hypotheses are defined as

$$\mathcal{H}_1 : U_J = 1,$n
$$\mathcal{H}_2 : U_J = 2.$$

Equivalently, $\mathcal{H}_1$ and $\mathcal{H}_2$ can also be described as the hypotheses that $Z_{1, J}$ is a member of the training set and $Z_{2, J}$ is a member of the training set, respectively. Denote $\pi_i = (\pi_{i, 1}, \pi_{i, 2})$ as a probability vector whose $i$-th element shows the belief of the prior at time $t$ that the true hypothesis is $\mathcal{H}_i$ for $i \in \{1, 2\}$. Then, we consider the prior as

$$P_i = N(\mu_{P_i}, \frac{2\eta_{\parallel d}}{\beta_{i-1}}),$$

where

$$\mu_{P_i} = W_{i-1} - \eta_{i-1} \frac{n-1}{n} \nabla \hat{R}_{S_i} (W_{i-1}) - \eta_{i-1} \frac{n}{n} \left( \pi_{i, 1} \nabla \ell(Z_{1, J}, W_{i-1}) + \pi_{i, 2} \nabla \ell(Z_{2, J}, W_{i-1}) \right).$$

\hspace{1cm} (57)

Here $\pi_i = (\frac{1}{2}, \frac{1}{2})$. Then, we construct the the belief vector $\pi_t$ for $t \geq 2$ using the log-likelihood ratio as

$$\pi_t = \left( \theta \log \frac{P_{\mathcal{F}_t}[\mathcal{H}_1]}{P_{\mathcal{F}_t}[\mathcal{H}_2]}, 1 - \theta \log \frac{P_{\mathcal{F}_t}[\mathcal{H}_1]}{P_{\mathcal{F}_t}[\mathcal{H}_2]} \right).$$

\hspace{1cm} (58)

where $\theta : \mathbb{R} \to [0, 1]$. Also, we might expect that the optimal $\theta$ satisfies $\theta(0) = \frac{1}{2}$, $\lim_{x \to -\infty} \theta(x) = 1$, and $\lim_{x \to -\infty} \theta(x) = 0$. 

13
Denote probability density function \( \mathbb{P}^{(2)}_{U,J,\mathcal{H}_I,W_0}[W_{1:T-1}] \) as \( f_k(W_{1:T-1}) \) for \( k \in \{1, 2\} \). Due to Markov structure of the update rule in Eq. (45), we have

\[
f_k(W_{1:T-1}) = \prod_{i=1}^{t-1} \left( \frac{\beta_{i-1}}{4\eta_{i-1}} \right)^{\frac{d}{2}} \exp \left( -\frac{\beta_{i-1} ||W_i - W_{i-1} + \eta_{i-1} \frac{n-1}{n} \nabla \tilde{R}_{S_i'}(W_{i-1}) + \frac{\eta_{i-1}}{n} \nabla \tilde{r}(Z_{i,j}, W_{i-1}) ||^2}{4\eta_{i-1}} \right).
\]  

(59)

Here, Eq. (59) is obtained by the Markov property of the update rule in Eq. (45). Then, since the prior distribution on \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) is uniform, we have

\[
\log \frac{\mathbb{P}^{(2)}_{U,J,\mathcal{H}_1}}{\mathbb{P}^{(2)}_{U,J,\mathcal{H}_2}} = \log \frac{f_1(W_{1:T-1})}{f_2(W_{1:T-1})}
= \sum_{i=1}^{t-1} (Y_{i,2} - Y_{i,1}),
\]

(60)

(61)

where \( Y_{i,1} \) and \( Y_{i,2} \) are given by

\[
Y_{i,1} = \sum_{i=1}^{t-1} \frac{\beta_{i-1}}{4\eta_{i-1}} ||W_i - W_{i-1} + \eta_{i-1} \frac{n-1}{n} \nabla \tilde{R}_{S_i'}(W_{i-1}) + \frac{\eta_{i-1}}{n} \nabla \tilde{r}(Z_{i,j}, W_{i-1}) ||^2,
\]

\[
Y_{i,2} = \sum_{i=1}^{t-1} \frac{\beta_{i-1}}{4\eta_{i-1}} ||W_i - W_{i-1} + \eta_{i-1} \frac{n-1}{n} \nabla \tilde{R}_{S_i'}(W_{i-1}) + \frac{\eta_{i-1}}{n} \nabla \tilde{r}(Z_{i,j}, W_{i-1}) ||^2.
\]

(62)

Therefore, the belief vector is given by

\[
\pi_t = \left( \theta \left( \sum_{i=0}^{t-1} (Y_{i,2} - Y_{i,1}) \right), 1 - \theta \left( \sum_{i=0}^{t-1} (Y_{i,2} - Y_{i,1}) \right) \right),
\]

(63)

where \( \pi_0 = Y_{0,2} = 0 \) and for \( t \geq 2 \), \( Y_{i,1} \) and \( Y_{i,2} \) are given by Eq. (62). To conclude the proof, we obtain

\[
\text{KL}(Q_t(S) \| P_t(\tilde{Z}^{(2)}, U_{J^*}, J)) \leq \sum_{t=1}^{T} \mathbb{E}^{(2)}_{U,J} \text{KL}(Q_t || P_t)
= \sum_{t=1}^{T} \mathbb{E}^{(2)}_{U,J} \beta_{i-1} \eta_{i-1} \left( (1 \{ U_j = 1 \} - \pi_{i,1}) \nabla \tilde{r}(Z_{i,j}, W_{i-1}) + (1 \{ U_j = 2 \} - \pi_{i,2}) \nabla \tilde{r}(Z_{i,j}, W_{i-1}) \right)^2
= \sum_{t=1}^{T} \mathbb{E}^{(2)}_{U,J} \beta_{i-1} \eta_{i-1} \left( (1 \{ U_j = 1 \} - \pi_{i,1})^2 ||\nabla \tilde{r}(Z_{i,j}, W_{i-1}) - \nabla \tilde{r}(Z_{i,j}, W_{i-1}) ||^2
\]

(64)

(65)

(66)

Finally, plugging Eq. (66) into Eq. (55), we get the desired result in Eq. (46).

\[
\begin{array}{c}
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14
\end{array}
\]
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A CMI and Fano’s Inequality

Let \( Z^{(k)} \), \( U \), and \( S \) as in Definition 1.2. Consider the following hypothesis testing problem. Assume a decision maker observes \( W \) bounded. Therefore, we can use the Hoeffding’s lemma to obtain the super-sample \( \tilde{Z}^{(k)} \). For any estimate \( \hat{U} = \Psi(W, \tilde{Z}^{(k)}) \), we have the Markov chain

\[
U \rightarrow S \rightarrow W \rightarrow \hat{U}.
\]

and so, combined with the fact that \( U \) is uniformly distributed over a set of size \( k^n \), we can invoke Fano’s inequality to bound the error probability of the decision maker. In particular,

\[
\inf_{\Psi} \mathbb{P}\left[ \Psi(W, \tilde{Z}^{(k)}) \neq U \right] \geq 1 - \frac{I(W; U|\tilde{Z}^{(k)}) + \log 2}{n \log k}.
\]

Hence, \( I(W; U|\tilde{Z}^{(k)}) \) provides a lower bound on the hardness of the hypothesis testing problem, where one wants to identify the training sample given access to \( \tilde{Z}^{(k)} \) and \( W \).

Some interpretation of our result is helpful. Consider an adversary who has access to the supersample \( \tilde{Z}^{(k)} \) and wishes to identify the training set that was used for the training after observing the output of a learning algorithm \( W \). Our result here showed that the CMI upperbounds the success probability of every adversary. Also, recall that the CMI upper bounds the expected generalization error. In the literature of data privacy in machine learning, this problem is known as Membership Attack (Shokri et al., 2017), and it is empirically observed that a machine learning model leaks information about its training set when the generalization error is large (Shokri et al., 2017). Our result in this section provide a formal connection between generalization and this specific membership attack problem.

B Proof of Theorem 4.3

For any two random measures \( P(\tilde{Z}^{(2)}, U_F, J) \) and \( Q(\tilde{Z}^{(2)}, U) \) on \( W \), the Donsker–Varadhan variational formula (Boucheron, Lugosi, and Massart, 2013, Prop. 4.15) and the disintegration theorem (Kallenberg, 2006, Thm. 6.4), give that with probability one

\[
\text{KL}(Q(\tilde{Z}^{(2)}, U) \| P(\tilde{Z}^{(2)}, U_F, J)) = \sup_{g \in \mathcal{G}} \left( Q(\tilde{Z}^{(2)}, U)[g] - \log P(\tilde{Z}^{(2)}, U_F, J)[\exp g] \right)
\]

where \( \mathcal{G} = \{ g : P(\tilde{Z}^{(2)}, U_F, J)(\exp g) < \infty \} \).

Let \( g = \frac{\lambda}{m} \sum_{j \in J} (-1)^j \ell(Z_{1,j}, W) - \ell(Z_{2,j}, W) \). First, note that

\[
\mathbb{E}^{\tilde{Z}^{(2)}, U_F, J} \left[ \frac{\lambda}{m} \sum_{j \in J} (-1)^j \ell(Z_{1,j}, W) - \ell(Z_{2,j}, W) \right] = 0.
\]

This is because \( \{ U_j \}_{j \in J} \) are independent of \( \tilde{Z}^{(2)}, U_F \), and \( J \). Moreover, \( g \) is \([-\lambda, \lambda]\)-bounded. Therefore, we can use the Hoeffding’s lemma to obtain

\[
\log P(\tilde{Z}^{(2)}, U_F, J)(\exp g) \leq \frac{\lambda^2}{2}.
\]

Hence, from Eq. (67), we conclude that

\[
Q(\tilde{Z}^{(2)}, U) \left[ \frac{1}{m} \sum_{j \in J} (-1)^j \ell(Z_{1,j}, W) - \ell(Z_{2,j}, W) \right] \leq \inf_{\lambda > 0} \frac{\text{KL}(Q(\tilde{Z}^{(2)}, U) \| P(\tilde{Z}^{(2)}, U_F, J))}{\lambda} + \frac{\lambda}{2} = \sqrt{2\text{KL}(Q(\tilde{Z}^{(2)}, U) \| P(\tilde{Z}^{(2)}, U_F, J))}
\]
almost surely. Finally, since $J \perp \tilde{Z}^2(U)$ we get

$$Q(\tilde{Z}^2(U)) \left[ \frac{1}{m} \sum_{j \in J} (-1)^j \left( \ell(Z_{1,j}, W) - \ell(Z_{2,j}, W) \right) \right]$$

$$= Q(\tilde{Z}^2(U)) \left[ \frac{1}{n} \sum_{i=1}^n (-1)^j \left( \ell(Z_1, W) - \ell(Z_2, W) \right) \right]$$

$$= \mathbb{E} \left[ R_D(W) - \hat{R}_S(W) \right]$$

The desired result follows.

### C Conditional Han’s Inequality

**Lemma C.1.** Let $(X_1, \ldots, X_n, Y)$ be $n+1$-dimensional random variable where $X_1, \ldots, X_N$ are discrete random variables. Then,

$$\frac{1}{k \binom{n}{k}} \sum_{T \in [n]_k} H(X_T | Y)$$

is decreasing in $k$.

**Proof.** For notational convenience, let $H_k(X_{[n]} | Y) = \frac{1}{(k)} \sum_{T \in [n]_k} H(X_T | Y)$. Note that if we manage to show that

$$H_k(X_{[n]} | Y) - H_{k-1}(X_{[n]} | Y) \leq H_{k+1}(X_{[n]} | Y) - H_k(X_{[n]} | Y), \quad (68)$$

then the result in Lemma C.1 follows. To show Eq. (68), we can write

$$H(X_1, \ldots, X_{k+1} | Y) + H(X_1, \ldots, X_{k-1} | Y)$$

$$= H(X_1, \ldots, X_k | Y) + H(X_{k+1} | X_1, \ldots, X_k, Y) + H(X_1, \ldots, X_{k-1} | Y) \quad (69)$$

$$\leq H(X_1, \ldots, X_k | Y) + H(X_{k+1} | X_1, \ldots, X_k-1, Y) + H(X_1, \ldots, X_{k-1} | Y) \quad (70)$$

$$= H(X_1, \ldots, X_k | Y) + H(X_1, \ldots, X_{k-1}, X_{k+1} | Y). \quad (71)$$

Here in Eq. (70), we drop $X_k$ from the condition in the second term. Therefore, we have

$$H(X_1, \ldots, X_{k+1} | Y) + H(X_1, \ldots, X_{k-1} | Y) \leq H(X_1, \ldots, X_k | Y) + H(X_1, \ldots, X_{k-1}, X_{k+1} | Y). \quad (72)$$

Then, by averaging Eq. (72) over all $n!$ permutation of $\{1, \ldots, n\}$, we get the desired result in Eq. (68).