UNDERSTANDING GENERALIZATION VIA LEAVE-ONE-OUT CONDITIONAL MUTUAL INFORMATION

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Abstract. We study the mutual information between (certain summaries of) the output of a learning algorithm and its $n$ training data, conditional on a supersample of $n + 1$ i.i.d. data from which the training data is chosen at random without replacement. These leave-one-out variants of the conditional mutual information (CMI) of an algorithm (Steinke and Zakynthinou, 2020) are also seen to control the mean generalization error of learning algorithms with bounded loss functions. For learning algorithms achieving zero empirical risk under 0–1 loss (i.e., interpolating algorithms), we provide an explicit connection between leave-one-out CMI and the classical leave-one-out error estimate of the risk. Using this connection, we obtain upper and lower bounds on risk in terms of the (evaluated) leave-one-out CMI. When the limiting risk is constant or decays polynomially, the bounds converge to within a constant factor of two. As an application, we analyze the population risk of the one-inclusion graph algorithm, a general-purpose transductive learning algorithm for VC classes in the realizable setting. Using leave-one-out CMI, we match the optimal bound for learning VC classes in the realizable setting, answering an open challenge raised by Steinke and Zakynthinou (2020). Finally, in order to understand the role of leave-one-out CMI in studying generalization, we place leave-one-out CMI in a hierarchy of measures, with a novel unconditional mutual information at the root. For 0–1 loss and interpolating learning algorithms, this mutual information is observed to be precisely the risk.

1. Introduction

In this paper, we study generalization in supervised learning. Formally, consider spaces of inputs $\mathcal{X}$, labels $\mathcal{Y}$, and classifiers $\mathcal{H} \subseteq \mathcal{Y}^\mathcal{X}$. Let $\mathcal{D}$ be a distribution on $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$. The empirical risk of a classifier $h : \mathcal{X} \to \mathcal{Y}$ on a sample $s = ((x_1, y_1), \ldots, (x_n, y_n)) \in \mathcal{Z}^n$ is $\hat{R}_n(h) = n^{-1} \sum_{i \in [n]} \ell(h, (x_i, y_i))$, where $\ell : \mathcal{Y}^\mathcal{X} \times \mathcal{Z} \to \mathbb{R}_+$ is the loss function. Let $S_n \sim \mathcal{D}^n$, i.e., let $S_n$ be a sequence of i.i.d. random elements in $\mathcal{Z}$ with common distribution $\mathcal{D}$. The risk of $h$ is $R_\mathcal{D}(h) = \mathbb{E}\hat{R}_{S_n}(h)$, where $\mathbb{E}$ denotes the expectation operator. A distribution $\mathcal{D}$ is said to be realizable by a class $\mathcal{H} \subseteq \mathcal{Y}^\mathcal{X}$ if $\inf_{h \in \mathcal{H}} R_\mathcal{D}(h) = 0$. Let $\mathcal{A} = (A_n)_{n \geq 1}$ denote a (potentially randomized) learning algorithm, which, for any positive integer $n$, maps $S_n$ to an element $A_n(S_n)$ of $\mathcal{Y}^\mathcal{X}$. We say $\mathcal{A}$ is an interpolating algorithm for datasets of size $n$ if $\hat{R}_{S_n}(A_n(S_n)) = 0$ a.s. If $\mathcal{A}$ is interpolating for all $n$, we say $\mathcal{A}$ is consistent. Our primary interest in this

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paper is the expected generalization error of $A_n$ with respect to $D$, defined as
\[
EGE_D(A_n) = \mathbb{E}[R_D(A_n(S_n)) - \hat{R}_{S_n}(A_n(S_n))],
\]
where we average over both the choice of training sample and the randomness within the algorithm $A_n$. Characterizing $EGE_D(A_n)$ provides us a handle on the performance of the learned classifier on unseen data. Note that, for interpolating algorithms, expected generalization error is expected risk, i.e.,
\[
EGE_D(A_n) = \mathbb{E}[R_D(A_n(S_n))] \triangleq R_D(A_n).
\]

Among the many contributions of learning theory are various frameworks for analyzing the generalization error of learning algorithms. Examples include uniform convergence and VC theory [2], stability [3], and differential privacy [4]. In recent years, there has been a flurry of interest in the use of information-theoretic quantities for characterizing the expected generalization error of learning algorithms. This line of work, initiated by Russo and Zou [5] and Xu and Raginsky [6], has been extended in many directions. The basic result is that the generalization error can be bounded in terms of the mutual information between the training data and the learned classifier. Unfortunately, this framework is provably unable to explain generalization in some settings [7–10]. For instance, Livni and Moran [9] show that, for the class of one-dimensional thresholds\(^1\) over $\{1, \ldots, m\}$, $m \in \mathbb{N}$, for every learning algorithm $A$, there exists a realizable distribution such that either the risk (population loss) is “large” or the mutual information scales as $\Omega(m)$, leading to vacuous generalization bounds. However, for the same problem, VC theory implies that the population risk of every empirical risk minimizer goes to zero at the rate of $O(1/n)$.

In order to overcome some of these limitations, Steinke and Zakynthinou [11] propose a modified information-theoretic framework, which they dub Conditional Mutual Information (CMI). In this framework, a “supersample” is introduced and the training set is obtained as a subsample. In particular, the supersample is a $2 \times n$ array, $\tilde{Z} \in \mathbb{Z}^{2 \times n}$, composed of i.i.d. samples from the data distribution $D$. Then, for an array $\tilde{U}$ independent from $\tilde{Z}$ and uniformly distributed in $\{0, 1\}^n$ (hence, $\tilde{U}$ is composed of i.i.d. Bernoulli random variables with mean $1/2$), the training set is $S_n = (\tilde{Z}_{\tilde{U}_{i,i}})_{i \in [n]}$. The conditional mutual information (CMI) of a learning algorithm $A_n$ on $n$ training data from $D$ is defined to be $I(A_n(S_n); \tilde{U} | \tilde{Z})$, i.e., the conditional mutual information of the output classifier $A_n(S_n)$ and $\tilde{U}$, conditioned on $\tilde{Z}$. In the same work, the authors also introduce the notion of the evaluated CMI of an algorithm, $I(L; \tilde{U} | \tilde{Z})$, where $L$ is the $2 \times n$ array of losses incurred by $A_n(S_n)$ on the supersample $\tilde{Z}$.

Results by Steinke and Zakynthinou [11], Haghifam et al. [12], and Harutyunyan et al. [13] show that CMI and its evaluated CMI (eCMI) counterpart provide an expressive framework for bounding generalization, encompassing multiple existing frameworks for proving generalization. Despite these results, it is not known whether the CMI/eCMI framework can be used to characterize minimax rates of expected risk in all circumstances. As one key example, it is not known

\(^1\)This concept class can be defined as follows. Let $\mathcal{X} = \{1, \ldots, m\}$. The class of one-dimensional thresholds over $\{1, \ldots, m\}$ is $\mathcal{H}_m = \{h_k | k \in \mathbb{N}\}$, where $h_k : \mathcal{X} \to \{0, 1\}$ is $h_k(x) = 1[x > k]$. 
whether any information-theoretic framework can obtain minimax rates for supervised classification problems with VC classes on realizable distributions.

1.1. Our Results. In this paper, we introduce a new information-theoretic measure of dependence between the output of a learning algorithm and its input, based on a leave-one-out analogue of eCMI:

**Definition 1.1.** Let \( \mathcal{A} \) be a learning algorithm. Let \( n \in \mathbb{N} \), let \( \tilde{Z} = (\tilde{Z}_i)_{i \in [n+1]} \) be an \( n+1 \)-array of i.i.d. random elements in the dataspace \( Z \) with common distribution \( \mathcal{D} \). Let \( U \) be a random variables distributed uniformly on \([n+1]\), independent from \( \tilde{Z} \). For \( u \in [n+1] \), let \( \tilde{Z}_{-u} \) denote \((\tilde{Z}_j)_{j \in [n+1], j \neq u}\), i.e., the supersample with the \( u \)'th element removed. Define \( S_n = \tilde{Z}_{-U} \). Let \( L \in \mathbb{R}^{n+1} \) be the array with entries \( L_i = \ell(\mathcal{A}_n(S_n), \tilde{Z}_i) \) for \( i \in [n+1] \). The leave-one-out (evaluated) conditional mutual information of \( \mathcal{A}_n \) with respect to \( \mathcal{D} \) is

\[
\text{LOO}^c\text{CMI}_D(\mathcal{A}_n) \triangleq I(L; U | \tilde{Z}.
\]

Our notion is inspired by the *leave-one-out error* estimator of the generalization error [14], a widely used surrogate for the expected generalization error. Intuitively, \( \text{LOO}^c\text{CMI}_D(\mathcal{A}_n) \) measures how well one can “identify” which point from the supersample is being held-out, given the supersample and the losses incurred on each of its elements. In Section 2, we show that bounded \( \text{LOO}^c\text{CMI}_D(\mathcal{A}_n) \) implies generalization in both interpolating and agnostic learning algorithms. Our generalization bound for the interpolating case enjoys the property that it is never greater than one.

In Section 3, in the context of 0–1 loss and interpolating learning algorithms, we establish a general connection between \( \text{LOO}^c\text{CMI} \) and the classical leave-one-out error estimator of the risk. Using this result, we show that \( \text{LOO}^c\text{CMI}_D(\mathcal{A}_n) \) precisely characterizes the risk of interpolating learning algorithms in many common situations. Specifically, we show that, for every data distribution and interpolating learner, the \( \text{LOO}^c\text{CMI}_D(\mathcal{A}_n) \) framework yields a risk bound that vanishes *if and only if* the risk also vanishes as the number training samples diverges. Also, the \( \text{LOO}^c\text{CMI}_D(\mathcal{A}_n) \) framework is the first information-theoretic framework that can be shown to determine the risk of any consistent learning algorithms whose risk either converge to a non-zero value or converges to zero polynomially with the number of samples.

In Section 4, as an application of our general connection with leave-one-out error analysis, we characterize the \( \text{LOO}^c\text{CMI} \) of the one-inclusion graph algorithm, which was introduced by Haussler et al. [15] for learning Vapnik–Chervonenkis (VC) classes. Using our framework, we obtain the *optimal* risk bound for every VC class in the realizable setting. In doing so, we answer the open problem stated in [16] of characterizing the expected excess risk of learning VC classes using an information-theoretic framework.

In Section 5, we consider several additional measures of information based on the supersample structure introduced in Definition 1.1, show that they all control generalization, and discuss their inter-relationships. In particular, we present the chain of inequalities

\[
I(L; U) \leq I(L; U | \tilde{Z}) \leq I(\tilde{Y}; U | \tilde{Z}) \leq I(\mathcal{A}_n(S_n); U | \tilde{Z}) \leq I(\mathcal{A}_n(S_n); S_n),
\]

(1)
where $I(\mathcal{A}_n(S_n); U|\tilde{Z})$ is the non-evaluated analogue of our notion and $\tilde{Y}$ is the length-$n + 1$ list of labels predicted by $\mathcal{A}_n(S_n)$ on the inputs in the supersample $\tilde{Z}$. With the exception of the first quantity, $I(L; U)$, all of these (or close analogues) have been studied in the literature. In the special case of binary classification by an interpolating classifier, $I(L; U)$ is precisely the risk, yielding a simple argument for why the other notions also bound risk (equivalently, generalization error) in this setting. Based on results presented herein and elsewhere, we discuss gaps between these various notions in Eq. (1) and the roles they can play in understanding generalization. In particular, we show that LOO-CMI is the weakest measure in this chain that can characterize the risk for every interpolating algorithm under 0–1 loss.

1.2. Related Work. For supervised learning algorithms, Steinke and Zakynthinou [11, Sec. 6] and Harutyunyan et al. [13] define information-theoretic measures of dependence based on the losses and predictions, respectively, of a learning algorithm rather than the learned classifier. The results in both of these papers are based on the CMI framework, i.e., a supersample with $2n$ samples. Neither of these papers recover optimal bounds for learning VC classes in the realizable setting. Hafez-Kolahi et al. [17] combine chaining with CMI to study generalization of deterministic learning algorithms. For ERM on classes of finite VC dimension $d$ in the agnostic case, i.e., $\inf_{h \in \mathcal{H}} R_D(h) \neq 0$, Hafez-Kolahi et al. use chaining CMI to obtain bounds on the expected generalization error that achieve the optimal rate $O(\sqrt{d/n})$. See also [18–26].

1.3. Notation. Let $P, Q$ be probability measures. For a $P$-integrable function $f$, let $P[f] = \int f dP$. When $Q$ is absolutely continuous with respect to $P$, denoted $Q \ll P$, write $\frac{dQ}{dP}$ for (an arbitrary version of) the Radon–Nikodym derivative (or density) of $Q$ with respect to $P$. The KL divergence (or relative entropy) of $Q$ with respect to $P$, denoted $\text{KL}(Q \parallel P)$, is defined as $Q[\log \frac{dQ}{dP}]$ when $Q \ll P$ and infinity otherwise.

For a random element $X$ in some measurable space $\mathcal{X}$, let $\mathbb{P}[X]$ denote its distribution, which lives in the space $\mathcal{M}_1(\mathcal{X})$ of all probability measures on $\mathcal{X}$. Given another random element, say $Y$ in $\mathcal{T}$, let $\mathbb{P}^Y[X]$ denote the conditional distribution of $X$ given $Y$. If $X$ and $Y$ are independent, denoted by $X \perp \perp Y$, we have $\mathbb{P}^Y[X] = \mathbb{P}[X]$ a.s.

The mutual information between $X$ and $Y$ is $I(X; Y) = \text{KL}(\mathbb{P}[(X, Y)] \parallel \mathbb{P}[X] \otimes \mathbb{P}[Y])$, where $\otimes$ forms the product measure. Writing $\mathbb{P}^Z[(X, Y)]$ for the conditional distribution of the pair $(X, Y)$ given a random element $Z$, the disintegrated mutual information between $X$ and $Y$ given $Z$, is $I^Z(X; Y) = \text{KL}(\mathbb{P}^Z[(X, Y)] \parallel \mathbb{P}^Z[X] \otimes \mathbb{P}^Z[Y])$, and the conditional mutual information is $I(X; Y|Z) = \mathbb{E}[I^Z(X; Y)|Z]$. Similarly, we can define disintegrated entropy of $X$ given $Y$ denoted by $H^Y(X)$, and its expectation gives the conditional entropy of $X$ given $Y$, i.e., $H(X|Y) = \mathbb{E}[H^Y(X)]$.

2. Generalization Bounds

In this section, we show that bounded LOO-CMI implies generalization. First, we provide a generalization bound for interpolating learning algorithms:
Theorem 2.1. Let $n \in \mathbb{N}$, assume loss is bounded in $[0,1]$, and let $A_n$ be an interpolating learning algorithm. Then,

$$R_D(A_n) \leq \frac{\text{LOO}^c\text{CMI}_D(A_n)}{\log(n+1)}.$$

Remark 2.2. By the definition of mutual information, $\text{LOO}^c\text{CMI}_D(A_n) \leq H(U|\tilde{Z}) \leq \log(n+1)$, since $U \perp \perp \tilde{Z}$ and $U$ is distributed uniformly on $[n+1]$. Therefore, the bound above is never greater than one. ▷

Proof of Theorem 2.1. Let $D$, $\tilde{Z}$, $U$, and $L$ be defined as in Definition 1.1. Introduce $\tilde{U}$ such that $\tilde{U} \overset{d}{=} U$ and $\tilde{U} \perp \perp (\tilde{Z},L)$. By the Donsker–Varadhan variational formula [27, Prop. 4.15], for all bounded measurable functions $h$ and $\lambda \in \mathbb{R}$,

$$I(\tilde{Z}, L; U) = \text{KL}(\mathbb{P}(\tilde{Z}, U, L) \| \mathbb{P}(\tilde{Z}, L) \otimes \mathbb{P}(\tilde{U}))$$

$$\geq \mathbb{P}(\tilde{Z}, U, L)(\lambda h) - \log \left( \left( \mathbb{P}(\tilde{Z}, L) \otimes \mathbb{P}(\tilde{U}) \right)(\exp(\lambda h)) \right).$$

Let $\alpha \in \mathbb{R}_+$ be a constant. Consider the function $h_\alpha : \mathbb{Z}^{n+1} \times [n+1] \times [0,1]^{n+1} \to \mathbb{R}$ given by $h_\alpha(\tilde{z}, u, l) = l_u - \alpha \sum_{i \in [n+1], i \neq u} l_i$. Then

$$\mathbb{P}(\tilde{Z}, U, L)(h_\alpha) = \mathbb{E}[\mathbb{E}^U h_\alpha(U, L, \tilde{Z})]$$

$$= \mathbb{E}[\mathbb{E}^U \left( \ell(A_n(\tilde{Z}_u-U), \tilde{Z}_U) - \alpha \sum_{i \in [n], i \neq U} \ell(A_n(\tilde{Z}_u-U), \tilde{Z}_i) \right)]$$

$$\overset{(a)}{=} \mathbb{E}[\mathbb{E}^U \left( \ell(A_n(\tilde{Z}_u-U), \tilde{Z}_U) \right)]$$

$$= \mathbb{E}[R_D(A_n(S_u))] = R_D(A_n(S_u)).$$

Here, $(a)$ follows from the fact that $A_n$ is an interpolating algorithm, hence, for all $i \neq U$, $\ell(A_n(\tilde{Z}_u-U), \tilde{Z}_i) = 0$ a.s. Thus, by Eq. (2), Eq. (3), and $I(L, \tilde{Z}; U) = \text{LOO}^c\text{CMI}_D(A_n)$, we obtain

$$R_D(A_n) \leq \frac{\text{LOO}^c\text{CMI}_D(A_n)}{\lambda}$$

$$+ \frac{\log \left( \left( \mathbb{P}(\tilde{Z}, L) \otimes \mathbb{P}(\tilde{U}) \right)(\exp(\lambda h_\alpha)) \right)}{\lambda}.$$
To simplify the notation, let \( \ell(i, j) = \ell(A_n(\tilde{Z}_{-i}), \tilde{Z}_j) \) for \( i \) and \( j \) in \( [n+1] \). We have
\[
\mathbb{P}(\tilde{Z}, L) \otimes \mathbb{P}(\tilde{U}) \left( \exp(\lambda h_{\alpha}) \right)
\]
\[
\overset{(a)}{=} \mathbb{E} \left[ \exp \left[ \lambda(\ell(U, \tilde{U}) - \alpha \sum_{i \in [n+1], i \neq \tilde{U}} \ell(U, i)) \right] \right]
\]
\[
= \mathbb{E} \left[ 1[U = \tilde{U}] \exp \left[ \lambda(\ell(U, \tilde{U}) - \alpha \sum_{i \in [n+1], i \neq \tilde{U}} \ell(U, i)) \right] \right]
\]
\[
+ \mathbb{E} \left[ 1[U \neq \tilde{U}] \exp \left[ \lambda(\ell(U, \tilde{U}) - \alpha \sum_{i \in [n+1], i \neq \tilde{U}} \ell(U, i)) \right] \right]
\]
\[
\overset{(b)}{=} \mathbb{E} \left[ 1[U = \tilde{U}] \exp(\lambda \ell(U, U)) \right] + \mathbb{E} \left[ 1[U \neq \tilde{U}] \exp(-\lambda \alpha \ell(U, U)) \right] + \mathbb{E} \left[ \frac{1}{n+1} \exp(\lambda \ell(U, U)) + \frac{n}{n+1} \exp(-\lambda \alpha \ell(U, U)) \right].
\]
The equality \((a)\) follows from the chain rule. In particular, the expectation over \( \tilde{Z} \) and \( L \) can be written as \( \mathbb{E}\mathbb{E}\tilde{Z},U \). Step \((b)\) follows from the fact that for all \( i \in [n+1] \) and \( i \neq U \), \( \ell(U, i) = 0 \) a.s., since the algorithm is interpolating. In \((c)\) we take the expectation with respect to \( \tilde{U} \) and use the fact that \( \tilde{U} \) is independent of \( \tilde{Z}, U \), and the internal randomness of \( A \). Let \( \lambda = \log(n+1) \). Consider the function \( f : [0, 1] \rightarrow \mathbb{R} \), where \( f(x) = \frac{1}{n+1} \exp(\lambda x) + \frac{n}{n+1} \exp(-\lambda \alpha x) \). Note that \( f \) is the sum of two convex functions, defined on a bounded domain. It achieves its maximum over the endpoint, i.e., \( x \in \{0, 1\} \). Considering this observation, we can further upper bound Eq. \((5)\) by considering the following two cases: If \( \ell(U, U) = 1 \), then \( \frac{\exp(\lambda \ell(U, U)) + n \exp(-\lambda \alpha \ell(U, U))}{n+1} = 1 + \frac{n}{n+1} \exp(-\alpha \log(n+1)) \). Otherwise, in the case that \( \ell(U, U) = 0 \), we have
\[
\frac{\exp(\lambda \ell(U, U)) + n \exp(-\alpha \log(n+1))}{n+1} = 1.
\]
Therefore, we conclude
\[
\mathbb{P}(\tilde{Z}, L) \otimes \mathbb{P}(\tilde{U}) \left( \exp(\lambda h_{\alpha}) \right) \leq 1 + \frac{n}{n+1} \exp(-\alpha \log(n+1)).
\]
By Eq. \((4)\) and Eq. \((6)\)
\[
R_D(A_n) \leq \frac{I(L; U | \tilde{Z}) + \log \left( 1 + \frac{n \exp(-\alpha \log(n+1))}{n+1} \right)}{\log(n+1)}.
\]
Finally, letting \( \alpha \rightarrow +\infty \) in Eq. \((7)\) concludes the proof. \( \square \)

**Remark 2.3.** The special case of zero–one loss can be proven in a more direct way. See Section 5. \( \diamond \)

**Remark 2.4.** In this remark, we consider a seemingly more elementary argument to establish Theorem 2.1, but show that the logic underlying this approach is flawed. Assume that the loss function is zero–one loss and that the algorithm is interpolating. In this setup, note that \( H^L,Z(U) = 0 \) almost surely on the event \( L \neq (0, \ldots, 0) \). The reason is that the algorithm can make an error only on the test point in \( \tilde{Z} \). Therefore, we can write \( I(L; U | \tilde{Z}) = H(U | \tilde{Z}) - H(U | L, \tilde{Z}) = H(U | L) \).
\[
\log(n + 1) - \mathbb{E}\left[ H^{L,Z}(U) \mathbb{1}[L = (0,\ldots,0)] \right].
\]

One’s intuition might suggest that, conditional on the event \( L = (0,\ldots,0) \), there is no mutual information between \( U \) and \((\tilde{Z}, L)\). One might then leap to
\[
\mathbb{E}\left[ H^{L,Z}(U)|L = (0,\ldots,0) \right] = \log(n + 1),
\]
from which one would reason that
\[
I(L; U|\tilde{Z}) = \log(n + 1) - \log(n + 1)(1 - R_D(A_n)) = R_D(A_n) \log(n + 1).
\]

However, the intuition is flawed. Consider the class of thresholds in one dimension. In Fig. 1, we consider learning from \( n = 4 \) data, when the supersample is in a neighborhood of a sequence \((z_1,\ldots,z_5)\). Given the training data \( S_n \), let \( x^* = \max\{x|(x,1) \in S_n\} \) if \( S_n \) contains at least one point with label 1, otherwise let \( x^* = -\infty \). Consider the learning algorithm \( A_n(S_n) = \hat{h} \) where \( \hat{h}(x) = \mathbb{1}[x \leq x^*] \). On the event \( L = (0,\ldots,0) \) and \( \tilde{Z} \) is a small perturbation of the points \((z_1,\ldots,z_5)\), we have \( \mathbb{P}^{L,Z}[U = 3] = 0 \). The reason is, had it been the case that \( U = 3 \), then the learning algorithm would have erred on its prediction for (the point corresponding to) \( z_3 \). Therefore,
\[
\mathbb{E}\left[ H^{L,Z}(U)|L = (0,\ldots,0) \right] \neq \log(n + 1), \text{ in general.} \]

For an arbitrary learning algorithm, LOO^cCMI still controls generalization. The proof of the following theorem is deferred to Section 5.

**Theorem 2.5.** Let \( n \in \mathbb{N} \). Assuming only that loss is bounded in \([0,1]\),
\[
\text{EGE}_D(A_n) \leq \sqrt{2\text{LOO}_D^c\text{CMI}(A_n)}.
\]

### 3. A Connection with leave-one-out error

In this section, we describe a connection between LOO^cCMI and the leave-one-out error, a well-studied statistical estimator of risk [28, 29]. Using the supersample \( \tilde{Z} \), the random variable
\[
\hat{R}_{\text{loo}} = \frac{1}{n + 1} \sum_{i=1}^{n+1} \mathbb{E}[\tilde{Z}(\hat{h}(A_n(\tilde{Z}_i), Z_i)]
\]
is a leave-one-out error estimate for the risk of \( A_n \), where we have averaged out the internal randomness in \( A_n \). (Note that, for deterministic learning algorithms, this averaging has no effect.) In order to connect this quantity to LOO^cCMI, we first note that we can bound LOO^cCMI\(_D(A_n)\) in terms of the disintegrated entropy:
\[
(8) \quad \text{LOO}_D^c\text{CMI}(A_n) = \mathbb{E}\left[ H^{\tilde{Z}}(L) - H^{\tilde{Z},U}(L) \right] \leq \mathbb{E}\left[ H^{\tilde{Z}}(L) \right],
\]
where the second inequality is an equality for deterministic learning algorithms. Let \( H_b(\cdot) \) denote the binary entropy function.
\textbf{Theorem 3.1.} Let $A_n$ be an interpolating learning algorithm for some data distribution $\mathcal{D}$. Assume loss lies in $\{0,1\}$. Then, almost surely,

\begin{equation}
H^{\tilde{Z}}(L) \leq H_b(\hat{R}_{\text{loo}}) + \hat{R}_{\text{loo}} \log (n + 1) \tag{9}
\end{equation}

\textit{Proof.} Let $0(0) = (0, \ldots, 0) \in \{0,1\}^{n+1}$ and, for $i \in \{1, \ldots, n+1\}$, let $0(i) \in \{0,1\}^{n+1}$ be equivalent to $0(0)$ but for a 1 at index $i$. Due to interpolation, the support of $L$ is $\{0(i)|i \in \{0, \ldots, n+1\}\}$. For each $i, j \in \{1, \ldots, n+1\}$, let

$$\kappa_{i,j} = \mathbb{P}^{\tilde{Z}, U = j}[L = 0(i)] = \mathbb{P}^{\tilde{Z}}[\ell(A_n(\tilde{Z} - j), \tilde{Z}) = 1].$$

Since $A_n$ is a consistent algorithm $\kappa_{i,j} = 0$ a.s. for $i \neq j$. Also, $\mathbb{E}[\kappa_{i,i}] = R_D(A_n)$. For $i \in \{1, \ldots, n+1\}$,

$$\mathbb{P}^{\tilde{Z}}[L = 0(i)] = \mathbb{E}^{\tilde{Z}}[\mathbb{P}^{\tilde{Z}, U}[L = 0(i)]] = \frac{1}{n+1} \sum_{j=1}^{n+1} \kappa_{i,j} = \frac{\kappa_{i,i}}{n+1},$$

where the last line follows since $\kappa_{i,j} = 0$ for $i \neq j$. Note that the leave-one-out-error satisfies $\hat{R}_{\text{loo}} = (n+1)^{-1} \sum_{i=1}^{n+1} \kappa_{i,i}$. Then, by the definition of the entropy,

$$H^{\tilde{Z}}(L) = - \sum_{i=0}^{n+1} \mathbb{P}^{\tilde{Z}}[L = 0(i)] \log \mathbb{P}^{\tilde{Z}}[L = 0(i)]$$

\begin{equation}
= -(1 - \hat{R}_{\text{loo}}) \log (1 - \hat{R}_{\text{loo}}) - \sum_{i=1}^{n+1} \frac{\kappa_{i,i}}{n+1} \log \left( \frac{\kappa_{i,i}}{n+1} \right) \tag{10}
\end{equation}

We now invoke the log-sum inequality for non-negative sequences $\{a_i\}_{i \in [n]}$ and $\{b_i\}_{i \in [n]}$, wherein $\sum_{i=1}^{n} a_i \log \frac{a_i}{b_i} \geq (\sum_{i \in [n]} a_i) \log \frac{\sum_{i \in [n]} a_i}{\sum_{i \in [n]} b_i}$. Using this inequality, we obtain

\begin{equation}
\sum_{i=1}^{n+1} \frac{\kappa_{i,i}}{n+1} \log \left( \frac{\kappa_{i,i}}{n+1} \right) \geq \hat{R}_{\text{loo}} \log \left( \frac{\hat{R}_{\text{loo}}}{n+1} \right) \tag{11}
\end{equation}

Therefore, by Eqs. (10) and (11),

$$H^{\tilde{Z}}(L) \leq -(1 - \hat{R}_{\text{loo}}) \log (1 - \hat{R}_{\text{loo}})$$

$$- \hat{R}_{\text{loo}} \log \hat{R}_{\text{loo}} + \hat{R}_{\text{loo}} \log (n+1)$$

$$= H_b(\hat{R}_{\text{loo}}) + \hat{R}_{\text{loo}} \log (n+1),$$

as was to be shown. \hfill \Box

As a corollary, we provide an explicit bound on LOO-CMI.

\textbf{Corollary 3.2.} Let $A_n$ be a consistent learning algorithm for zero–one valued loss, let $\mathcal{D}$ be a distribution on $\mathcal{Z}$, and assume that, with probability one,
\[ \hat{R}_{\text{loo}} \leq \frac{\theta}{n+1}, \] where \( \theta \) is some \( \tilde{Z} \)-measurable random variable in \( \mathbb{R}_+ \). Then, almost surely,

\[
I^{\tilde{Z}}(L; U) \leq \begin{cases} 1 + \frac{\theta \log(n+1)}{2n+1} + \frac{\theta + \exp(-1)}{n+1}, & \text{if } \frac{\theta}{n+1} \geq \frac{1}{2}, \\ \frac{\theta}{n+1}, & \text{otherwise}. \end{cases}
\]

Proof. For the case \( 2\theta \geq n+1 \), upper-bounding the \( H_b(\hat{R}_{\text{loo}}) \) by one, we obtain the result. For the case \( 2\theta < n+1 \), note that \( H_b(x) \leq -x \log(x) + x \), we obtain

\[
I^{\tilde{Z}}(L; U) \leq \frac{\theta}{n+1} \log(n+1) + \frac{\theta}{n+1} + \frac{\theta \log(n+1)}{n+1} \]

where the last line follows from \( \max_{x>0} -x \log(x) = \exp(-1) \). \( \square \)

Corollary 3.2 can be used to obtain risk bound for a variety of consistent learning algorithms. For example, the Support Vector Machine (SVM) algorithm has a leave-one-out error guarantee in the sense of Corollary 3.2 for realizable distributions, where \( \theta \) is given by the number \( N_{\text{SV}}(\tilde{Z}) \) of support vectors in the supersample \( \tilde{Z} \) [14]. Therefore, assuming \( D \) is a realizable distribution with respect to the class of half-spaces in \( \mathbb{R}^d \), the LOO-CMI of the SVM satisfies

\[
\text{LOO}^c\text{CMI}_D(A_n) \leq \frac{\mathbb{E}[N_{\text{SV}}(\tilde{Z})]}{n+1} (2\log(n+1) + 1).
\]

Combining this result with Theorem 2.1 yields a bound on the risk of SVM that is optimal up to a constant factor [30].

3.1. Universality of LOO\textsuperscript{c}CMI. In this section, we demonstrate that leave-one-out CMI captures the asymptotics of risk for consistent learners. More precisely, for every data distribution \( D \) and consistent learner \( A \), the quantity \( \text{LOO}^c\text{CMI}_D(A_n)/\log(n+1) \) vanishes as the number training samples \( n \) diverges if and only if the risk also vanishes. Also, for a broad class of learning algorithms for which the population risk converges to zero polynomially in the size of the training set, \( \text{LOO}^c\text{CMI}_D(A_n)/\log(n+1) \) vanishes at the same rate as \( R_D(A_n) \).

Theorem 3.3. Let \( A_n \) be an interpolating learning algorithm for some data distribution \( D \). Assume loss lies in \( \{0, 1\} \). Then,

\[
\text{LOO}^c\text{CMI}_D(A_n) \leq H_b(R_D(A_n)) + R_D(A_n) \log(n+1)
\]

and

\[
R_D(A_n) \log(n+1) \leq \text{LOO}^c\text{CMI}_D(A_n).
\]
Proof. Since the binary entropy function is concave, it follows from Jensen’s inequality, Theorem 3.1, and the identity \( \mathbb{E}[\hat{R}_{\text{loo}}] = R_D(A_n) \) that
\[
H(L|\hat{Z}) = \mathbb{E}[H(\hat{Z}(L)] \\
\leq \mathbb{E}[H_b(\hat{R}_{\text{loo}}) + \hat{R}_{\text{loo}} \log(n + 1)] \\
\leq H_b(R_D(A_n)) + R_D(A_n) \log(n + 1),
\]
which was to be shown. Finally, the lower bound (Eq. (13)) is Theorem 2.1. □

Remark 3.4. Are these bounds tight for consistent learners in the large n limit? First consider the case that the risk of \( A_n \) does not converge to zero as \( n \) diverges, i.e., \( R_D(A_n) = \Theta(1) \). Then \( \text{LOO}\text{CMI}_D(A_n)/\log(n + 1) = \Theta(R_D(A_n)) \). For consistent learning algorithms such that \( R_D(A_n) = c \frac{\log(n)^{\alpha}}{n^\beta} \) where \( c, \alpha \) and \( \beta \) are some non-negative constants, we claim that \( \text{LOO}\text{CMI}_D(A_n)/\log(n + 1) = \Theta(R_D(A_n)) \). This claim follows by bounding Eq. (12) using the well-known inequality \( H_b(p) \leq -p \log(p) + p \) for \( p \in [0, 1] \).

Remark 3.5. Let \( X = [0, 1] \) and \( Y = \{0, 1\} \). The class of (right-continuous) one-dimensional thresholds over \( X \) is \( \mathcal{H} = \{h_\theta \mid \theta \in X\} \) where \( h_\theta(x) = 1[x > \theta] \). Consider a continuous realizable distribution \( D \) for \( \mathcal{H} \) with positive margin, i.e., the data labelled 0 and 1 are separated by an interval. For any proper algorithm, we may write \( A(S_n) = h_{\hat{\theta}} \) for some random variable \( \hat{\theta} \) in \( X \). Using the margin assumption, we can design \( A \) so that (1) \( h_{\hat{\theta}} \) achieves zero training error yet (2) the representation of \( \hat{\theta} \) encodes the whole training set, in the sense that, having \( \hat{\theta} \) and \( \hat{Z} \), we can decode \( U \) perfectly. For this algorithm, we then have \( I(A(S_n); U|\hat{Z}) = \log(n + 1) \). On the other hand, for this class, [31] showed that any algorithm with zero training error achieves \( R_D(A_n) = O(1/n) \). Therefore, our result in Theorem 3.3 shows that \( I(L; U|\hat{Z})/\log(n + 1) = O(1/n) \). This example separates \( I(L; U|\hat{Z}) \) and \( I(A(S_n); U|\hat{Z}) \), and served as motivation for Definition 1.1. As we discuss elsewhere, if sufficiently tight control on generalization can be obtained via a formally looser bound, doing so yields an stronger explanation. □

4. AN OPTIMAL BOUND FOR LEARNING VC CLASSES

We start this section with some standard definitions [32]. Consider binary classification, i.e., \( Y = \{0, 1\} \), with zero–one loss. A sequence \((x_1, y_1, \ldots, x_n, y_n)\) is said to be realizable by \( \mathcal{H} \), if for some \( h \in \mathcal{H} \), \( h(x_i) = y_i \) for all \( i \in [n] = \{1, \ldots, n\} \). Note that, if \( D \) is realizable by \( \mathcal{H} \), then, for all \( n \in \mathbb{N} \), the sequence \( S_n \sim D^n \) is a.s. realizable by \( \mathcal{H} \). We say \( \mathcal{H} \) shatters \((x_1, \ldots, x_m) \in X^m \) if for all \((y_1, \ldots, y_m) \in \{0, 1\}^m \), there exists \( h \in \mathcal{H} \), such that, for all \( i \in [m] \), we have \( h(x_i) = y_i \). The VC dimension of \( \mathcal{H} \), denoted \( d \), is the supremum of integers \( m \geq 0 \) for which there exists \((x_1, \ldots, x_m) \in X^m \) shattered by \( \mathcal{H} \). In particular, if there is no largest such integer, the VC dimension is infinite, i.e., \( d = \infty \).

In this section, we study the \( \text{LOO}\text{CMI} \) of the classical one-inclusion graph algorithm, which was first proposed by Haussler et al. [15] as a general-purpose transductive learner for VC classes in the realizable setting. Here, we provide a brief description of this algorithm. Let \( \mathcal{H} \) be a class with a
bounded VC dimension. Assume a realizable sequence of \( n \) labeled samples \( S_n = ((x_1, y_1), \ldots, (x_n, y_n)) \in \mathcal{Z}^n \) and a test point \( x_{n+1} \) is given to the learner, and the learner is tasked to predict the label of \( x_{n+1} \). Let \( V \) be the set of all possible labelings of \( (x_1, \ldots, x_{n+1}) \) by the classifiers in \( \mathcal{H} \), i.e., \( V = \{ (v_1, \ldots, v_{n+1}) \in \{0, 1\}^{n+1} \mid \exists h \in \mathcal{H}, \forall i \in [n+1], h(x_i) = v_i \} \). The one-inclusion graph \([15]\) is the graph with vertex set \( V \) such that vertices \( \vec{v}, \vec{w} \in V \) are connected by an edge if and only if the Hamming distance between \( \vec{v} \) and \( \vec{w} \) is one. A probability assignment \( P \) is a function \( P : V \times V \rightarrow [0, 1] \) such that (i) \( P(\vec{v}, \vec{w}) > 0 \) only if \( \vec{v} \) and \( \vec{w} \) are adjacent (in particular, \( P(\vec{v}, \vec{v}) = 0 \) for all \( \vec{v} \in V \)) and (ii) given two adjacent vertices \( \vec{v} \) and \( \vec{w} \), we have \( P(\vec{v}, \vec{w}) + P(\vec{w}, \vec{v}) = 1 \). We assume that \( P \) is chosen based only on \((x_1, \ldots, x_{n+1})\), i.e., independently of the labels.

We say a vertex \( \vec{v} = (v_1, \ldots, v_{n+1}) \in V \) is consistent with the labels in \( S_n \) if \( (v_1, \ldots, v_n) = (y_1, \ldots, y_n) \). Since the labels of \((x_1, \ldots, x_n)\) are known, Haussler et al. \([15]\) observed that at most two vertices in the one-inclusion graph are consistent with the labels in \( S_n \). In the case that only vertex \( \vec{v} = (v_1, \ldots, v_{n+1}) \in V \) is consistent with \( S_n \), the label of \( x_{n+1} \) is predicted as \( v_{n+1} \). In the case that two vertices \( \vec{v} = (v_1, \ldots, v_{n+1}) \) and \( \vec{w} = (w_1, \ldots, w_{n+1}) \) are consistent with \( S_n \), they differ only on the \((n+1)\)-th position and the algorithm uses the probability assignment \( P \) to predict that the label for \( x_{n+1} \) agrees with \( v_{n+1} \) with probability \( P(\vec{v}, \vec{w}) \) and agrees with \( w_{n+1} \) otherwise.

Consider a realizable distribution \( \mathcal{D} \) and let \( h^* \in \mathcal{H} \) denote a function that determines the labels. Haussler et al. \([15]\) prove that the leave-one-out error of the one-inclusion graph algorithm can be expressed in terms of the probability assignment \( P \) as

\[ \hat{R}_{\text{loo}} = \frac{\sum_{\vec{v} \in V} P(\vec{h}^*, \vec{v})}{n+1}, \]

where \( \vec{h}^* = (h^*(X_1), \ldots, h^*(X_{n+1})) \in V \) is the vertex corresponding to \( h^* \) in the one-inclusion graph of \((X_1, \ldots, X_{n+1})\). Moreover, Haussler et al. \([15]\) prove that there exists a probability assignment \( P \) such that \( \sum_{\vec{v} \in V} P(\vec{w}, \vec{v}) \leq d \) uniformly over all \( \vec{w} \in V \). By combining this result and Theorem 4.1, we obtain the main result of this section.

**Theorem 4.1.** Let \( \mathcal{A} \) denote the one-inclusion graph algorithm. Then, for every VC class \( \mathcal{H} \) with dimension \( d \), every data distribution \( \mathcal{D} \) realizable by \( \mathcal{H} \), and \( n \geq d \), there exists a probability assignment for the one-inclusion graph algorithm such that \( \text{LOO-CMI}_D(\mathcal{A}_n) \leq \frac{d}{n+1}(2\log(n+1) + 1) \). Combining this result with the generalization bound in Theorem 2.1 yields expected risk \( \frac{2d}{n+1}(1 + o(1)) \) which is optimal up to a constant factor \([33]\).

Using our general reduction (Theorem 3.1), we have characterized the LOO-CMI of the one-inclusion graph algorithm and, as a consequence, shown that the LOO-CMI framework provides an optimal bound for learning VC classes. It is worth noting that the IOMI framework of Russo and Zou \([5]\) and Xu and Raginsky \([6]\) is provably unable to characterize the learnability of VC classes \([9]\), and, at present, the best known bound within the CMI framework \([11]\) is suboptimal by a \( \log(n) \) factor \([16]\).
5. A Hierarchy of Measures of Information

We have introduced leave-one-out CMI and shown that it can be used to bound the expected generalization error of learning algorithms. In this section, we aim to relate leave-one-out CMI to other measures of mutual information, some of which have already been shown to control generalization.

To begin, we place leave-one-out CMI in a chain of inequalities:

\[
I(L; U) \overset{(a)}{\leq} I(L; U|\tilde{Z}) \overset{(b)}{\leq} I(\hat{Y}; U|\tilde{Z}) \overset{(c)}{\leq} I(A_n(S_n); U|\tilde{Z}) \overset{(d)}{\leq} I(A_n(S_n); S_n).
\]  

Fig. 2 presents the conditional independence relationsihps that hold among the various random variables we have introduced. In the chain of inequalities, (a) follows from the fact that \( U \perp \tilde{Z} \); (b), (c) follow from the data-processing inequality; and (d) is shown by Haghifam et al. [34]. Except for the first quantity, \( I(L; U) \), each quantity, or some close analogue, has been studied in the literature. For example, \( I(\hat{Y}; U|\tilde{Z}) \) was studied by Harutyunyan et al. [13] in the context of CMI with a supersample of size \( 2n \). Indeed, the same sequence of inequalities hold for the analogous \( 2n \)-supersample quantities in the CMI framework.

We now show that \( I(L; U) \) exactly determines the risk (equivalently, expected generalization error) of consistent algorithms for 0–1 loss. For bounded loss functions, \( I(L; U) \) upper-bounds the generalization error of arbitrary learning algorithms.

**Theorem 5.1.** Let \( D \) be a distribution on \( \mathcal{Z} \) and let \( A_n \) be a learning algorithm for \( n \in \mathbb{N} \) i.i.d. data. For any \([0, 1]\)-bounded loss function,

\[
\text{EGE}_D(A_n) \leq \sqrt{2I(L; U)}.
\]

If \( A_n \) is almost surely interpolating, then, for zero–one loss,

\[
R_D(A_n) = \frac{I(L; U)}{\log(n + 1)}.
\]

**Proof.** Consider a \([0, 1]\)-bounded loss. For all \( i \in [n + 1] \), let \( \rho_i : [n + 1] \to \mathbb{R} \) be

\[
\rho_i(j) = \begin{cases} 
1 & \text{if } j = i, \\
-\frac{1}{n} & \text{otherwise}.
\end{cases}
\]
Let $\mathcal{D}, \tilde{Z}, U, L,$ and $\tilde{U}$ be as in the proof of Theorem 2.1. By the Donsker–Varadhan variational formula [27, Prop. 4.15], for all bounded measurable functions $h$ and for all $\lambda \in \mathbb{R}$

$$I(L; U) = \text{KL}(\mathbb{P}(U, L) \parallel \mathbb{P}(L) \otimes \mathbb{P}(\tilde{U}))$$

(15)

$$\geq \mathbb{P}(U, L)(\lambda h) - \log \left[ (\mathbb{P}(L) \otimes \mathbb{P}(\tilde{U}))(\exp(\lambda h)) \right].$$

Consider now the function $h : [n + 1] \times [0, 1]^{n+1} \to [-1, 1]$ given by $h(u, l) = \sum_{i=1}^{n+1} \rho_i(u)l_i$. Then

$$\mathbb{P}(U, L)(h) = \mathbb{E}[\mathbb{E}^U[h(U, L)]]$$

$$= \mathbb{E}[\mathbb{E}^U[\ell(\mathcal{A}_n(\tilde{Z}-U), \tilde{Z}_U) - \frac{1}{n} \sum_{i \in [n], i \neq U} \ell(\mathcal{A}_n(\tilde{Z}-U), \tilde{Z}_i)]]$$

$$= \mathbb{E}[\mathbb{R}_D(\mathcal{A}_n(S_n)) - \mathbb{R}_S(\mathcal{A}_n(S_n)))]$$

(16)

$$= \mathbb{E}\mathbb{G}D(\mathcal{A}_n).$$

Moreover, for all $i \in [n+1]$, we have $\mathbb{E}[\rho_i(\tilde{U})] = 0$. Therefore $\mathbb{E}^L h(\tilde{U}, L) = 0$ since $\tilde{U} \perp \perp L$. Using Hoeffding’s lemma and the fact that $|h| \leq 1$, we obtain

(17) $\mathbb{P}(L) \otimes \mathbb{P}(\tilde{U})(\exp(\lambda h)) = \mathbb{E}[\mathbb{E}^L \exp(\lambda h(\tilde{U}, L))] \leq \exp(\lambda^2/2).$

By Eqs. (15) to (17), $\mathbb{E}\mathbb{G}D(\mathcal{A}_n) \leq \frac{I(L; U)}{\lambda} + \frac{1}{2}$. Finally, letting $\lambda = \sqrt{2I(L; U)}$, we obtain the stated result.

Now consider 0–1 loss and assume $\mathcal{A}_n$ is interpolating. By the definition of the mutual information, we have $I(L; U) = H(L) - H(L|U)$. Let $0_{(i)}$, $i \in \{0, \ldots, n+1\}$ be as in the proof of Theorem 3.3. Because $\mathcal{A}_n$ is interpolating, the support of $L$ is $\{0_{(i)}|i \in \{0, \ldots, n+1\}\}$. For $i > 0$,

$$\mathbb{P}(L = 0_{(i)}) = \frac{1}{n + 1} \mathbb{P}(\ell(\mathcal{A}_n(\tilde{Z}-i), \tilde{Z}_i) = 1) = \frac{R_D(\mathcal{A}_n)}{n + 1},$$

where we have used the fact that $R_D(\mathcal{A}_n) = \mathbb{P}(\ell(\mathcal{A}_n(\tilde{Z}-i), \tilde{Z}_i) = 1)$ for $i > 0$. Therefore,

$$H(L) = -\sum_{i=0}^{n+1} \mathbb{P}(L = 0_{(i)}) \log(\mathbb{P}(L = 0_{(i)}))$$

(18)

$$= -(1 - R_D(\mathcal{A}_n)) \log(1 - R_D(\mathcal{A}_n)) - R_D(\mathcal{A}_n) \log \frac{R_D(\mathcal{A}_n)}{n + 1}.$$ 

Similarly, we have

$$H(L|U) = \frac{1}{n + 1} \sum_{i=1}^{n+1} H_{U=i}(L)$$

(19)

$$= -(1 - R_D(\mathcal{A}_n)) \log(1 - R_D(\mathcal{A}_n)) - R_D(\mathcal{A}_n) \log R_D(\mathcal{A}_n).$$

Using Eq. (18), Eq. (19), and the definition of the mutual information, the stated result follows.

**Remark 5.2 (Proof of Theorem 2.5).** From Theorem 5.1 and the inequality $I(L; U) \leq I(L; U|\tilde{Z})$, we obtain Theorem 2.5.
Remark 5.3 (Maximal gaps). Using the fact that \( I(\mathcal{A}_n(S_n); U|\tilde{Z}) \leq H(U) \leq \log(n+1) \), Theorem 5.1 and Eq. (14) imply that, for 0–1 loss and interpolating learning algorithms, we have

\[
R_D(\mathcal{A}_n) = \frac{I(L; U)}{\log(n+1)} \leq \frac{I(L; U|\tilde{Z})}{\log(n+1)} \leq \frac{I(\hat{Y}; U|\tilde{Z})}{\log(n+1)} \leq \frac{I(\mathcal{A}_n(S_n); U|\tilde{Z})}{\log(n+1)} \leq 1.
\]

Starting from this chain of inequalities, we can investigate the gap between these different measures of dependency. Of course, the maximal (additive) gap between all these measures is \( \log(n+1) \). Is this gap achieved?

- **\( I(\hat{Y}; U|\tilde{Z}) \) versus \( I(\mathcal{A}_n(S_n); U|\tilde{Z}) \):** Note that, for binary classification under 0–1 loss, we have \( I(L; U|\tilde{Z}) = I(\hat{Y}; U|\tilde{Z}) \). This is due to \( L \) being a one-to-one function of \( \tilde{Z} \) and \( \hat{Y} \). As shown in Remark 3.5, there is a maximal gap between \( I(L; U|\tilde{Z}) \) and \( I(\mathcal{A}_n(S_n); U|\tilde{Z}) \). Therefore, there exists a learning scenario in which \( I(\mathcal{A}_n(S_n); U|\tilde{Z}) = \Omega(\log(n+1)) \) while \( I(\hat{Y}; U|\tilde{Z}) \in o(\log(n+1)) \).

- **\( I(L; U|\tilde{Z}) \) versus \( I(\hat{Y}; U|\tilde{Z}) \):** Consider a setting where \( \mathcal{X} = \mathcal{Y} = [-1, 1] \) and the loss function is \( \ell(\hat{y}, (x, y)) = \mathbb{1}[\hat{y}y < 0] \). Let the data distribution be that of \( (X, h^*(X)) \), where \( X \) is uniformly distributed on \( \mathcal{X} \) and \( h^*(x) = \mathbb{1}[x > 0] \). Consider the learning rule \( \mathcal{A}_n(S_n)(x) = y \) where \( (x, y) \in S_n \) and \( \mathcal{A}_n(S_n)(x) = x \) otherwise. This algorithm is consistent by design and the expected risk of this algorithm is zero. Therefore, Theorem 3.3 and Theorem 5.1 show that \( I(L; U) = I(L; U|\tilde{Z}) = 0 \). However, it can be easily seen that \( I(\hat{Y}; U|\tilde{Z}) = \log(n+1) \). Thus there exists a learning scenario such that there is a maximal gap between \( I(\hat{Y}; U|\tilde{Z}) \) and \( I(L; U|\tilde{Z}) \).

- **\( I(L; U) \) versus \( I(L; U|\tilde{Z}) \):** Our result in Theorem 3.3 shows that the gap between these two quantities cannot be maximal. Also, as mentioned in Remark 3.4, for learning algorithms whose expected risk decays polynomially in \( n \) to zero, \( I(L; U) \) can only be tighter than \( I(L; U|\tilde{Z}) \) by a constant factor. Note that since \( I(L; U) \log(n+1) \) is the risk, any characterization of the gap between \( I(L; U) \) and \( I(L; U|\tilde{Z}) \) is the same as characterization of the gap between \( I(L; U|\tilde{Z}) \) and the risk. Understanding the exact gap between these two measures is important future work.

\[\checkmark\]

**Remark 5.4.** One advantage of working with \( I(L; U|\tilde{Z}) \) and \( I(\hat{Y}; U|\tilde{Z}) \), over non-evaluated LOO CMI \( I(\mathcal{A}_n(S_n); U|\tilde{Z}) \), is that the former quantities do not require one to have a parametrization of the set of possible classifiers. Of course, the training data themselves always serve as a “parametrization” for nonrandomized learning rules, but such a parameterization leads to vacuous bounds. (The same roadblocks pertain to plain CMI.) A quintessential example of a setting where natural parametrization may not exist is that of transductive learning algorithms, i.e., ones whose input includes the test input and whose output is the corresponding label prediction. The \( k \)-Nearest Neighbor Algorithm is one specific example. \[\checkmark\]
Remark 5.5. The leave-one-out CMI framework provides numerous estimates of the expected generalization error based on various measures of information. Which measure should one use to understand generalization? To simplify the discussion, let us focus on the case of interpolating learners under 0–1 loss, in which case expected generalization error is simply risk. Theorem 5.1 indicates that \( I(L;U) \) is equal to the risk. As such, there appears to be no advantage to studying \( I(L;U) \). Of course, once one recognizes that risk is a mutual information, one can invoke information-theoretic results to obtain quantities that may be easier to estimate, such as provided by the bound \( I(L;U) \leq I(L;U|\tilde{Z}) \).

Even if one can directly bound or compute \( I(L;U) \), there may be advantages to studying measures that are never tighter, such as the quantities later in the chain of inequalities in Eq. (14). As argued by Dziugaite et al. [35], if a formally looser quantity controls generalization error (or risk) to a sufficient extent, then this looser quantity provides a more general explanation of the empirical generalization phenomena, as the adequacy of any formally tighter bound is then tautological. That is, when attempting to explain generalization phenomena, use the loosest bound that suffices.

This perspective also suggests that identifying tighter bounds should not be the goal of studying generalization from an information-theoretic perspective. Instead, we seek a rich hierarchy of bounds and an understanding of their interrelationships, so that we can come to understand generalization in specific instances in terms of the level in this hierarchy needed to explain the phenomenon.

Besides the challenge of identifying the right quantity to explain a phenomenon of interest, there are statistical and computational barriers to studying generalization. The measures of information presented here and studied by other authors all depend on the data distribution, which in many interesting settings is not known, other than through a random sample. Even in cases where certain distributions are known, many of these quantities are computationally intractable, without exploiting special structure. There are ways to navigate around these roadblocks. One example is demonstrated by work using “data-dependent estimates” to study generalization in iterative algorithms in deep learning [36, 34, 37].

6. Conclusion

We have presented a leave-one-out variant of the CMI framework, a novel information-theoretic framework to reason about generalization in machine learning. For 0–1 loss and interpolating learning algorithms, LOO$^c$CMI provides upper and lower bounds on risk. For consistent learners that are interpolating for any number of data, the LOO$^c$CMI framework captures the asymptotics of risk when the risk converges to a nonzero quantity or to zero polynomially. As an application of the LOO$^c$CMI framework, we have studied the leave-one-out CMI of the one-inclusion graph algorithm [15], and shown that the framework yields an optimal risk bound for learning VC classes in the realizable setting.
At present, it is not known whether optimal bounds for this setting can be achieved via any other existing information-theoretic framework.

**Open problems.** Our work raises several open problems:

1. Is Theorem 2.5 tight? In what settings (outside those of Theorem 3.3) can one obtain tighter bounds? In particular, can one use the leave-one-out CMI framework to obtain tight (up to universal constants) bounds on the generalization error of arbitrary algorithms, similar to what we showed for interpolating learning algorithms?

2. Is Theorem 3.3 tight for finite \( n \)? Under what conditions can we remove or tighten the binary entropy term?

3. Can one obtain an optimal bound for the one-inclusion graph algorithm under realizability via the standard CMI framework, or is there a lower bound? Is there any optimal (improper) learner for VC classes under realizability for which CMI yields optimal bounds? Lower bounds here would demonstrate that leave-one-out CMI is fundamentally stronger.

4. Leave-one-out CMI can be interpreted as an information-theoretic notion of stability. Are there connections to notions of algorithmic stability [38]?

In general, it is an open challenge to determine the \text{LOO}^{*}\text{CMI} of common learning algorithms to better understand this framework.

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**References**

[1] M. Haghifam, S. Moran, D. M. Roy, and G. K. Dziugaite. “Understanding Generalization via Leave-One-Out Conditional Mutual Information”. In: 2022 IEEE International Symposium on Information Theory (ISIT). 2022.

[2] V. Vapnik and A. Chervonenkis. Theory of pattern recognition. 1974.

[3] O. Bousquet and A. Elisseeff. “Stability and generalization”. Journal of Machine Learning Research 2.Mar (2002), pp. 499–526.

[4] C. Dwork, V. Feldman, M. Hardt, T. Pitassi, O. Reingold, and A. Roth. “Generalization in adaptive data analysis and holdout reuse”. In: Advances in Neural Information Processing Systems. 2015, pp. 2350–2358.
[5] D. Russo and J. Zou. “Controlling Bias in Adaptive Data Analysis Using Information Theory”. In: *Proceedings of the 19th International Conference on Artificial Intelligence and Statistics*. Ed. by A. Gretton and C. C. Robert. Vol. 51. Proceedings of Machine Learning Research. Cadiz, Spain: PMLR, 2016, pp. 1232–1240.

[6] A. Xu and M. Raginsky. “Information-theoretic analysis of generalization capability of learning algorithms”. In: *Advances in Neural Information Processing Systems*. 2017, pp. 2524–2533.

[7] R. Bassily, S. Moran, I. Nachum, J. Shafer, and A. Yehudayoff. “Learners that Use Little Information”. In: *Algorithmic Learning Theory*. 2018, pp. 25–55.

[8] I. Nachum, J. Shafer, and A. Yehudayoff. “A direct sum result for the information complexity of learning”. In: *Conference On Learning Theory*. PMLR. 2018, pp. 1547–1568.

[9] R. Livni and S. Moran. “A Limitation of the PAC-Bayes Framework”. In: *Advances in Neural Information Processing Systems*. Vol. 33. 2020, pp. 20543–20553.

[10] Y. Bu, S. Zou, and V. V. Veeravalli. “Tightening Mutual Information-Based Bounds on Generalization Error”. *IEEE Journal on Selected Areas in Information Theory* 1.1 (2020), pp. 121–130.

[11] T. Steinke and L. Zakynthinou. “Reasoning About Generalization via Conditional Mutual Information”. In: *Proceedings of the 33rd Conference On Learning Theory*. Ed. by J. Abernethy and S. Agarwal. Vol. 125. Proceedings of Machine Learning Research. PMLR, July 2020, pp. 3437–3452. arXiv: 2001.09122.

[12] M. Haghifam, G. K. Dziugaite, S. Moran, and D. Roy. “Towards a Unified Information-Theoretic Framework for Generalization”. *Advances in Neural Information Processing Systems* 34 (2021).

[13] H. Harutyunyan, M. Raginsky, G. Ver Steeg, and A. Galstyan. “Information-theoretic generalization bounds for black-box learning algorithms”. *Advances in Neural Information Processing Systems* 34 (2021).

[14] M. Mohri, A. Rostamizadeh, and A. Talwalkar. *Foundations of machine learning*. MIT press, 2018.

[15] D. Haussler, N. Littlestone, and M. K. Warmuth. “Predicting {0, 1}-functions on randomly drawn points”. *Information and Computation* 115.2 (1994), pp. 248–292.

[16] T. Steinke and L. Zakynthinou. “Open Problem: Information Complexity of VC Learning”. In: *Proceedings of the 33rd Conference On Learning Theory*. Ed. by J. Abernethy and S. Agarwal. Vol. 125. Proceedings of Machine Learning Research. PMLR, July 2020, pp. 3857–3863.

[17] H. Hafez-Kolahi, Z. Golgooni, S. Kasaei, and M. Soleymani. “Conditioning and Processing: Techniques to Improve Information-Theoretic Generalization Bounds”. In: *Advances in Neural Information Processing Systems* 34, 2020.

[18] G. Aminian, L. Toni, and M. R. Rodrigues. “Jensen-shannon information based characterization of the generalization error of learning algorithms”. In: *2020 IEEE Information Theory Workshop (ITW)*. IEEE. 2021, pp. 1–5.

[19] E. Clerico, A. Shidani, G. Deligiannidis, and A. Doucet. “Chained Generalisation Bounds”. arXiv preprint arXiv:2203.00977 (2022).

[20] R. Zhou, C. Tian, and T. Liu. “Individually Conditional Individual Mutual Information Bound on Generalization Error”. In: *2021 IEEE International Symposium on Information Theory (ISIT)*. 2021, pp. 670–675.
[21] H. Hafez-Kolahi, B. Moniri, and S. Kasaei. “Information-Theoretic Analysis of Minimax Excess Risk”. *arXiv preprint arXiv:2202.07537* (2022).

[22] I. Issa, A. R. Esposito, and M. Gastpar. “Strengthened Information-theoretic Bounds on the Generalization Error”. In: *2019 IEEE International Symposium on Information Theory (ISIT)*. 2019, pp. 582–586.

[23] J. Jiao, Y. Han, and T. Weissman. “Dependence measures bounding the exploration bias for general measurements”. In: *IEEE International Symposium on Information Theory*. 2017.

[24] A. Asadi, E. Abbe, and S. Verdú. “Chaining mutual information and tightening generalization bounds”. In: *Advances in Neural Information Processing Systems 32*. 2018.

[25] R. Zhou, C. Tian, and T. Liu. “Stochastic Chaining and Strengthened Information-Theoretic Generalization Bounds”. *arXiv preprint arXiv:2201.12192* (2022).

[26] B. Rodríguez-Gálvez, G. Bassi, R. Thobaben, and M. Skoglund. “On Random Subset Generalization Error Bounds and the Stochastic Gradient Langevin Dynamics Algorithm”. In: *IEEE Information Theory Workshop (ITW)*. IEEE. 2020.

[27] S. Boucheron, G. Lugosi, and P. Massart. *Concentration inequalities: A nonasymptotic theory of independence*. Oxford university press, 2013.

[28] T. M. Cover. “Learning in pattern recognition”. In: *Methodologies of pattern recognition*. Elsevier, 1969, pp. 111–132.

[29] M. Stone. “Cross-validatory choice and assessment of statistical predictions (with discussion)”. *Journal of the Royal Statistical Society: Series B (Methodological)* 38.1 (1976), pp. 102–102.

[30] P. M. Long and R. J. Long. “On the complexity of proper distribution-free learning of linear classifiers”. In: *Algorithmic Learning Theory*. PMLR. 2020, pp. 583–591.

[31] S. Hanneke. “Refined error bounds for several learning algorithms”. *The Journal of Machine Learning Research* 17.1 (2016), pp. 4667–4721.

[32] S. Shalev-Shwartz and S. Ben-David. *Understanding machine learning: From theory to algorithms*. Cambridge university press, 2014.

[33] Y. Li, P. M. Long, and A. Srinivasan. “The one-inclusion graph algorithm is near-optimal for the prediction model of learning”. *IEEE Transactions on Information Theory* 47.3 (2001), pp. 1257–1261.

[34] M. Haghifam, J. Negrea, A. Khisti, D. M. Roy, and G. K. Dziugaite. “Sharpened Generalization Bounds based on Conditional Mutual Information and an Application to Noisy, Iterative Algorithms”. In: *Advances in Neural Information Processing Systems*. 2020, pp. 9925–9935.

[35] G. K. Dziugaite, A. Drouin, B. Neal, N. Rajkumar, E. Caballero, L. Wang, I. Mitliagkas, and D. M. Roy. “In Search of Robust Measures of Generalization”. In: *Advances in Neural Information Processing Systems*. Vol. 33. 2020.

[36] J. Negrea, M. Haghifam, G. K. Dziugaite, A. Khisti, and D. M. Roy. “Information-Theoretic Generalization Bounds for SGLD via Data-Dependent Estimates”. In: *Advances in Neural Information Processing Systems*. 2019, pp. 11013–11023.

[37] H. Wang, Y. Huang, R. Gao, and F. Calmon. “Analyzing the Generalization Capability of SGLD Using Properties of Gaussian Channels”. *Advances in Neural Information Processing Systems* 34 (2021).

[38] A. Elisseeff, M. Pontil, et al. “Leave-one-out error and stability of learning algorithms with applications”. *NATO science series sub series iii computer and systems sciences* 190 (2003), pp. 111–130.