Conditional Mutual Information Bound for Meta Generalization Gap

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Abstract—Meta-learning infers an inductive bias—typically in the form of the hyperparameters of a base-learning algorithm—by observing data from a finite number of related tasks. This paper presents an information-theoretic upper bound on the average meta-generalization gap that builds on the conditional mutual information (CMI) framework of Steinke and Zakynthinou (2020), which was originally developed for conventional learning. In the context of meta-learning, the CMI framework involves a training meta-supersample obtained by first sampling 2N independent tasks from the task environment, and then drawing 2M independent training samples for each sampled task. The meta-training data fed to the meta-learner is then obtained by randomly selecting N tasks from the available 2N tasks and M training samples per task from the available 2M training samples per task. The resulting bound is explicit in two CMI terms, which measure the information that the meta-learner output and the base-learner output respectively provide about which training data are selected given the entire meta-supersample.

I. INTRODUCTION

In conventional learning, a learning algorithm uses training samples from an underlying unknown data distribution to infer a model parameter \( W \) from a model class \( \mathcal{W} \), so that the corresponding model performs well on a new data sample drawn from the same distribution. As formalized by the “no-free-lunch” theorem [1, Thm. 5.1], learning cannot take place without prior assumptions. These include assumptions on the model class \( \mathcal{W} \) and on the hyperparameters of the learning algorithm, such as learning rate and initialization, collectively known as inductive bias of the learning procedure. Conventionally, the inductive bias is determined on the basis of domain expertise and/or using validation with data from the same task. Meta-learning aims to automatically infer the inductive bias by observing data from a number of related tasks, so as to “speed up” the learning of a new, previously unseen task [2, 3].

The tasks observed in meta-learning are assumed to belong to a task environment \( \mathcal{H} \), which is defined by a distribution \( P_T \) over a set \( \mathcal{T} \) of tasks, and by a per-task data distributions \( \{P_{Z|T=t}\}_{t \in \mathcal{T}} \). A meta-learner observes meta-training data, consisting of randomly sampled data from a subset of tasks, where the tasks are in turn sampled from the task environment. The meta-training data is used to infer a hyperparameter vector \( u \), which specifies the inductive bias of a base learning algorithm. The goal of the meta-learner is to minimize the meta-generalization loss \( L(u) \), which is defined as the generalization (a.k.a. population) loss incurred by the hyperparameter \( u \) when used by the base-learner on a new task \( T \), generated independently from the meta-training tasks.

The meta-generalization loss is not computable by the meta-learner, since the task distribution \( P_T \) and the per-task data distributions \( \{P_{Z|T=t}\}_{t \in \mathcal{T}} \) are unknown. Instead, the meta-learner evaluates the empirical meta-training loss \( L_{Z_{1:N}}(u) \) for \( u \) based on the meta-training set \( Z_{1:N} \). The meta-training set consists of \( N \) training sets of \( M \) independent training samples each, with each set pertaining an independently generated task. The difference between the meta-generalization loss and the meta-training loss is the so-called meta-generalization gap. If the meta-generalization gap is small, on average or with high probability, the performance of the meta-learner on the meta-training set can be taken as a reliable measure of the meta-generalization loss.

Following the work of Russo and Zhou [5], information-theoretic bounds on the average generalization gap for conventional learning have been widely investigated in recent years [6–8]. The bounds in [6] depend on the mutual information (MI) between the output of the learning algorithm and the training set. In [7], a tighter bound is obtained by replacing this term with the MI between the algorithm output and each individual sample of the training set. Further refinements of these bounds involve computing the MI between the algorithm output and a random subset of the training data [8]. Some of these approaches have been extended to meta-learning in [9]. Relevant to this paper is the framework recently introduced in [10] for conventional learning, which will be referred to as conditional mutual information (CMI) framework. A key quantity in this framework is a supersample of \( 2M \) samples generated independently according to the underlying data distribution. The training samples fed to the learning algorithm are chosen by selecting \( M \) samples from the supersample at random. The bound on the average generalization gap reported in [10, Cor. 5.2] depends on the CMI between the algorithm output and the random vector that determines which training
data are selected from the supersample, given the supersample. Differently from MI-based bounds, the CMI-based bound given in [10] Cor. 5.2] is always bounded. In particular, it is non-vacuous for deterministic algorithms operating over continuous spaces.

Contributions: Inspired by [10], we present a novel information-theoretic bound on the average meta-generalization gap that extends the CMI-based bounds for conventional learning to meta-learning. Existing information-theoretic bounds on the meta-generalization gap [9] were instead derived using the MI and the individual-task MI approaches reviewed before. Other available bounds on the meta-generalization gap include Vapnik-Chervonenkis (VC)-dimension based probably-approximately-correct (PAC) bounds [4], and the PAC-Bayesian bounds in [11–13]. In line with [9], we show that there are two sources of generalization errors that contribute to the meta-generalization gap: (i) the environment-level meta-generalization gap, resulting from the observation of a finite number N of tasks; and (ii) the task-level generalization gap, resulting from the observation of a finite number M of data samples per task. Unlike prior work, these two contributions are quantified in our analysis via CMI terms that depend on a meta-supersample of per-task training data sets, from which a subset of tasks and per-task training data are randomly selected for use by the meta-learner and base-learners. The derived bound inherits the advantage of the CMI bound for conventional learning. Specifically, unlike the MI-based bounds of [9], it is bounded even when the meta-learner and the base-learner are deterministic algorithms operating on continuous spaces.

II. PROBLEM DEFINITION

In this section, we provide the key definitions for our setup.

A. Base-learner

Each task τ within some set of tasks T is associated with an underlying unknown data distribution P_{Z|T=τ} on a set Z. Throughout, sets can be discrete or continuous. For a given task τ_i, the base-learner observes a data set Z_i^M = (Z_{i,1}^M, ..., Z_{i,M}^M) of M independently and identically distributed (i.i.d.) samples from P_{Z|T=τ_i}. The base-learner uses the training set Z_i^M to infer a model parameter w ∈ W. We assume that the base-learner depends on an inductive bias that is defined by a hyperparameter vector u ∈ U. The performance of the model parameter w on a data sample z is measured by the loss function ℓ: W × Z → R^+. The goal of the base-learner is to infer the model parameter w ∈ W that minimizes the per-task generalization loss

$$L_{P_{Z|T=τ_i}}(w) = \mathbb{E}_{P_{Z|T=τ_i}}[\ell(w, Z)].$$

where the average is taken over a test sample Z ~ P_{Z|T=τ_i} drawn independently from Z_i^M. Since P_{Z|T} is unknown, the generalization loss L_{P_{Z|T=τ_i}}(w) cannot be computed. Instead, the base-learner evaluates the training loss

$$L_{Z_i^M}(w) = \frac{1}{M} \sum_{j=1}^{M} \ell(w, Z_j^M).$$

The difference between the generalization loss and the training loss is referred to as the generalization gap:

$$\Delta L(u|Z_i^M, u, τ_i) = L_{P_{Z|T=τ_i}}(w) - L_{Z_i^M}(w).$$

In this paper, we model the base-learner as a stochastic map P_{W|Z_i^M, u} from the input training data set Z_i^M to the model class W. As mentioned, this map depends on u.

B. Meta-Learner

The goal of meta-learning is to automatically infer the hyperparameter u of the base-learner P_{W|Z_i^M, u} from training data pertaining a number of related tasks. The tasks are assumed to belong to a task environment, which is defined by a task distribution P_T on the space of tasks T, and by the per-task data distributions \{P_{Z|T=τ}\}_{τ ∈ T}. The meta-learner observes a meta-training set Z_i^{1:N} = (Z_{i,1}, ..., Z_{i,N}) of N data sets. Each Z_i^M is generated independently by first drawing a task T_i ∼ P_T and then a task-specific dataset Z_i^M ∼ P_{Z|T=τ_i}. The meta-learner uses the meta-training set Z_i^{1:N} to infer the hyperparameter u. This is done with the goal of ensuring that, using the inferred hyperparameter u, the base-learner P_{W|Z_i^M, u} can efficiently learn on a new meta-test task T ∼ P_T given the corresponding training dataset Z_i^M.

Formally, the objective of the meta-learner is to infer the hyperparameter u that minimizes the meta-generalization loss

$$L(u) = \mathbb{E}_{P_T} P_{Z_i^M|T} \mathbb{E}_{P_{W|Z_i^M, u}}[L_{P_{Z|T}}(W)],$$

where the expectation is taken over an independently generated meta-test task T ∼ P_T, over the associated data set Z_i^M ∼ P_{Z|T=τ_i}, and over the output of the base-learner. Since P_T and \{P_{Z|T=τ}\}_{τ ∈ T} are unknown, the meta-generalization loss cannot be computed. Instead, the meta-learner can evaluate the meta-training loss, which for a given hyperparameter u, is defined as the average training loss on the meta-training set

$$L_{Z_i^{1:N}}(u) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_{P_{W|Z_i^M, u}}[L_{Z_i^M}(W)].$$

Here, the average is taken over the output of the base-learner. The difference between the meta-generalization loss and the meta-training loss is the meta-generalization gap

$$\Delta L(u|Z_i^{1:N}) = L(u) - L_{Z_i^{1:N}}(u).$$

Intuitively, if the meta-generalization gap is small, on average or with high probability, then the performance of the inferred hyperparameter u on the meta-training set can be taken as a reliable measure of the meta-generalization loss (4).
which maps the meta-training set $Z_{1:N}^M$ to the space of hyperparameters $\hat{U}$. We seek an information-theoretic upper bound on the average meta-generalization gap

$$\mathbb{E}_{P_{U|Z_{1:N}^M}}[\Delta L(U|Z_{1:N}^M)],$$

where $P_{U|Z_{1:N}^M} = P_{Z_{1:N}^M|U} P_U$ is the joint distribution of meta-training data and $\hat{U}$ induced by the meta-learner.

### III. A CMI-BASED FRAMEWORK FOR META-LEARNING

In this section, we introduce the CMI framework for meta-learning. We start by noting that the average meta-generalization gap \(7\) can be decomposed as \(9\)

$$\mathbb{E}_{P_{U|Z_{1:N}^M}}[\Delta L(U|Z_{1:N}^M)] = \mathbb{E}_{P_{U|Z_{1:N}^M}}[L(U) - \mathbb{E}_{P_{Z|2M}}[\hat{L}_{2M}(U)]] + \mathbb{E}_{P_{U|Z_{1:N}^M}}[\mathbb{E}_{P_{Z|2M}}[\hat{L}_{2M}(U)] - L_{2M}(U)], \quad (8)$$

where $\hat{L}_{2M}(u)$ denotes the average per-task training loss:

$$\hat{L}_{2M}(u) = \mathbb{E}_{P_{W|Z_{1:N},U}}[L_{2M}(W)]. \quad (9)$$

This quantity differs from the meta-training loss in that $U$ does not depend on the per-task training sets $Z_{1:N}^M$ used to evaluate the loss. On the contrary, the meta-training loss is evaluated on the meta-training data used to determine $\hat{U}$. It also differs from the meta-generalization loss, since it averages training losses and not test losses. The first expectation in \(8\) captures the average within-task generalization gap associated to meta-test task $T \sim P_T$, caused by the fact that only $M$ training samples per the task are available. The second expectation captures the average environment-level generalization gap, caused by the fact that the meta-learner observes only $N$ tasks.

To obtain an upper bound on the average meta-generalization gap, we bound these two expectations separately using the CMI approach introduced in the next section.

#### A. Per-Task Supersample and Meta-Supersamples

In this section, we define the per-task supersample following \(10\) and we introduce the concept of meta-supersample.

For a given task $\tau_i$, we define the per-task supersample as the collection $Z_{i}^{2M} = (Z_{i1}^{1}, \ldots, Z_{i}^{2M})$ of $2M$ samples draw independently from $P_{Z|T=\tau_i}$. Let $S_i = (S_i^1, \ldots, S_i^M)$ be an $M$-dimensional random vector whose elements are drawn independently from a Bernoulli distribution with parameter 0.5, independent of $Z_{i}^{2M}$. We use the vector $S_i$ to partition the per-task supersample $Z_{i}^{2M}$ into a set of $M$ input training samples fed to the base-learner, and a set of $M$ test samples. The vector of $M$ input training samples, which we denote as $\tilde{Z}_{i}^{2M}(S_i)$ is obtained as $\tilde{Z}_{i}^{2M}(S_i) = (Z_{i1}^{1+MS_i1}, Z_{i}^{2+MS_i2}, \ldots, Z_{i}^{M+MS_iM})$. Let $\bar{S}_i$ denote the vector whose entries are the modulo-2 complement of the entries of $S_i$. Then $\tilde{Z}_{i}^{2M}(\bar{S}_i)$ stands for the vector of test data for task $\tau_i$. We shall use the training sets $\tilde{Z}_{i}^{2M}(S_i)$ to train the base-learner, while the within-task generalization loss will be evaluated on the test data $Z_{i}^{2M}(\bar{S}_i)$.

We now describe the construction of the meta-supersample. We start by sampling $2N$ tasks, $T_1, \ldots, T_{2N}$, independently from $P_T$. For each $T_i$, we generate a per-task supersample $Z_{i}^{2M}$ as detailed above. The meta-supersample is then defined as $\tilde{Z}_{1:2N}^{2M} = (\tilde{Z}_{1}^{2M}, \ldots, \tilde{Z}_{2N}^{2M})$. Let now $R = (R_1, \ldots, R_N)$ be a $N$-dimensional random vector whose elements are drawn independently according to a Bernoulli distribution with parameter 0.5, independent of $\tilde{Z}_{1:2N}^{2M}$. We use the random vector $R$ to partition the meta-supersample into $N$ meta-training task datasets, and $N$ meta-test datasets. Specifically, the meta-training task datasets $\tilde{Z}_{i}^{2M}(R_1, \ldots, \tilde{Z}_{N}^{2M}(R_N))$ are obtained by setting $\tilde{Z}_{i+1}^{2M}(R_i) = \tilde{Z}_{i+1}^{2M}(R_i)$ for $i = 1, \ldots, N$. Finally, the meta-training data fed to the meta-learner is $\tilde{Z}_{1:2N}^{2M}(R, S_{1:N}) = (\tilde{Z}_{1}^{2M}(R_1, S_1), \ldots, \tilde{Z}_{N}^{2M}(R_N, S_N))$, where $\tilde{Z}_{i}^{2M}(R_i, S_i) = \tilde{Z}_{i}^{2M}(S_i)$. As before we let $\mathcal{B}$ be the vector whose entries are the modulo-2 complement of the entries of $R$, and use $\tilde{Z}_{1:2N}^{2M}(\mathcal{B})$ to denote all elements of $\tilde{Z}_{1:2N}^{2M}$ that are not in $\tilde{Z}_{1:2N}^{2M}(R)$. To sum up, the meta-training set $\tilde{Z}_{1:2N}^{2M}(R, S_{1:N})$ is generated by first choosing $N$ tasks from the meta-supersample $\tilde{Z}_{1:2N}^{2M}$ according to $R$, and then choosing $M$ samples per task from $\tilde{Z}_{i}^{2M}$ according to $S_i$, for $i = 1, \ldots, N$. Fig. 1 shows an example of meta-supersample.

#### IV. CMI-BASED BOUNDS ON AVERAGE META-GENERALIZATION GAP

In this section, we introduce a CMI-based bounds on the average meta-generalization gap. Throughout, we assume that the loss function $\ell(\cdot, \cdot)$ is bounded, i.e., $0 \leq a \leq \ell(\cdot, \cdot) \leq b < \infty$. As discussed in Section III, to obtain an upper bound on the average meta-generalization gap, we upper-bound separately the within-task and the environment-level generalization gaps. Towards this, we leverage the exponential-inequality-based approach introduced in \(14\).

#### A. Main Result

The main result of this paper is given below.

**Theorem 1:** Under the assumption that the loss function is bounded as $0 \leq a \leq \ell(\cdot, \cdot) \leq b < \infty$, the following bound on
the meta-generalization gap holds \( \tilde{\Delta} \):

\[
E_{U \sim \bar{Z}_{1:N}}[\tilde{\Delta}L(U|\bar{Z}_{1:N}^M)] 
\leq \sqrt{\frac{2(b-a)^2I(U; R, S_{1:N}|\bar{Z}_{1:2N}^M)}{N}} + \frac{1}{N} \sum_{i=1}^{N} \sqrt{2(b-a)^2\left(\frac{I(W; S_{i}|\bar{Z}_{1:2N}^M, R_{i})}{M}\right)}. \tag{10}
\]

The theorem is proved using exponential inequalities that we report in the next subsection, with details provided in Appendix B. The first term in \( \text{(10)} \) accounts for the environment-level generalization gap via the CMI \( I(U; R, S_{1:N}|\bar{Z}_{1:2N}^M) \) divided by the number \( N \) of meta-training tasks. The CMI \( I(U; R, S_{1:N}|\bar{Z}_{1:2N}^M) \) measures the information the meta-learner output reveals about the environment-level partition \( R \) and per-task partition \( S_{1:N} \) of the meta-supersample \( \bar{Z}_{1:2N}^M \), when the supersample \( Z_{1:2N}^M \) is given. The second term in \( \text{(10)} \) accounts for the within-task generalization gap through the CMI \( I(W; S_{i}|\bar{Z}_{1:2N}^M, R_{i}) \). Consistent with the per-task generalization gap bounds of \( \text{(10)} \), this second term measures the information the base-learner output reveals about the partitioning \( S_{i} \) of the per-task supersample \( Z_{1:2N}^M, R_{i} \), when the per-task supersample \( Z_{1:2N}^M, R_{i} \) is known.

The CMI-based bound \( \text{(10)} \) can be tighter than the MI-based bound on the average meta-generalization gap reported in \( [9] \) Eq. (34). In particular, following the notation in \( [9] \) and setting \( \sigma = \delta_k = (b-a)/2 \) in \( [9] \) Cor. 5.6 to account for the boundedness of the loss function in our setup, by a direct comparison of the two bounds we find that the CMI-based meta-learning bound is tighter than the \( \tilde{\Delta} \) meta-learning bound if the inequalities \( I(W; Z^M) > 3I(W; S|Z^M) \) and \( I(U; Z^M, R, S_{1:N}|Z^M, R_{1:N}) > 3I(U; R, S_{1:N}|Z^M, R_{1:N}) \) hold. More generally, a comparison between the MI and individual MI bounds derived in \( [9] \), should be done on a case-by-case basis.

The CMI-based bound \( \text{(10)} \) recovers the CMI bound for conventional learning in \( [10] \) Cor. 5.2 as special case. For conventional learning, the hyperparameter \( u \) is fixed \textit{a priori}. Moreover, the task environment can be assumed to be a delta function centered at some task \( \tau \in \mathcal{T} \), and the meta-training set with \( N = 1 \) reduces to the training set of task \( \tau \). Consequently, the first MI in \( \text{(10)} \) is zero, and \( \text{(10)} \) reduces to

\[
E_{P_{W \sim Z^M}}[\tilde{\Delta}L(W|Z^M)] 
\leq \sqrt{\frac{2(b-a)^2I(W; S|Z^M)}{M}}, \tag{11}
\]

which recovers the bound in \( [10] \) Cor. 5.2.

\[ \Box \]

### B. Exponential Inequalities

The proof of Theorem \( \text{I} \) relies on exponential inequalities that are used to bound the two terms in the decomposition \( \text{I} \). We detail these key technical results in this section.

We start by expressing the within-task generalization gap, \textit{i.e.,} the first expectation in the decomposition \( \text{I} \), in the following equivalent form, which makes explicit its dependence on the per-task supersamples and meta-supersample.

\[
E_{P_{U \sim \bar{Z}_{1:N}^M}}[L(U) - E_{P_{R \sim Z^M}}[\tilde{L}_Z(U)]]
= E_{P_{U \sim \bar{Z}_{1:N}^M}}E_{P_{R \sim Z^M}}E_{P_{W \sim Z^M}}[a_{\{\tilde{L}_Z(W) - L_Z(U)\}]} \tag{12}
= E_{P_{U \sim \bar{Z}_{1:N}^M}}E_{P_{R \sim Z^M}}E_{P_{W \sim Z^M}}[a_{\{L_{Z^M}(R, S_{1:N})\}}] \tag{13}
= \frac{1}{N} \sum_{i=1}^{N} E_{P_{W \sim Z^M}}[a_{\{L_{Z^M}(R_i, S_{i})\}}] \tag{14}
\]

The first equality \( \text{(13)} \) holds since the meta-learner is trained on the meta-supersamples \( \bar{Z}_{1:2N}(R, S_{1:N}) \), and since the average over \( P_{R \sim Z^M} \) in \( \text{(12)} \) can be evaluated on the independent test data set \( \bar{Z}_{1:2N}(R, S_{1:N}) \). Note that the sets \( Z^M(R, S_{1:N}) \) and \( \bar{Z}_{1:2N}(R, S_{1:N}) \) represent independent datasets from two different environment-level tasks, even if they share the same \( S_{1:N} \). Finally, we obtain \( \text{(14)} \) by taking the expectation inside the sum and by marginalizing over \( U \).

To keep notation compact, let the term within the average in \( \text{(14)} \) be defined as

\[
\tilde{\Delta}L(W, \bar{Z}_{1:2N}^M, R_{i}, S_{i}) = L_{Z^M}(R_i, S_{i}) - L_{Z^M}(R_{i}, S_{i}) \tag{15}
\]

We now present a task-level exponential inequality that will be useful to bound the expectation of this term. For generality, the bound is expressed in terms of the Radon–Nikodym derivatives of the relevant distributions (see, e.g., \( [13] \) Sec. 17.1).

**Proposition 1:** For all \( \lambda \in \mathbb{R} \), the following exponential inequality holds

\[
E_{P_{W \sim Z^M}}[a_{\{\lambda \tilde{\Delta}L(W, \bar{Z}_{1:2N}^M, R_{i}, S_{i})\}}] 
\leq \frac{\lambda^2(b-a)^2}{2M} \tag{16}
\]

where \( i(W; S|\bar{Z}_{1:2N}^M, R) \) is the conditional information density

\[
i(W; S|\bar{Z}_{1:2N}^M, R) = \log \frac{dP_{W \sim Z^M}(\bar{Z}_{1:2N}^M, R) \cdot P_S}{dP_{W \sim \bar{Z}_{1:2N}^M, R} \cdot P_S} \tag{16}
\]

**Proof:** See Appendix A. \( \Box \)

We now derive a similar exponential inequality to bound the average environment-level generalization gap, \textit{i.e.,} the second expectation on the right-hand side of \( \text{I} \). Let

\[
\tilde{\Delta}L(U, \bar{Z}_{1:2N}^M, R, S_{1:N}) 
= \tilde{L}_{Z^M}(R, S_{1:N})(U) - L_{Z^M}(R, S_{1:N})(U) \tag{17}
\]
where $L_{z^m, (u)}$ was defined in [5]. Using [17], and following steps similar to the ones leading to (14), we can express the environment-level generalization gap as

$$\mathbb{E}_{P_{U, z^m}} \left[ \mathbb{E}_{P_T, z^m} \left[ L_{z^m}(U) \right] - \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_{z^m_i} \right] = \mathbb{E}_{P_{U, z^m}, r_{1:N}, P_{U, z^m}, r_{1:N}} \left[ \tilde{\Delta} L(U, \hat{z}^m_{1:2N}, R, S_{1:N}) \right].$$  

(18)

In the next proposition, we state the relevant exponential inequality. The proof is similar to that of Proposition 1 and, hence, omitted.

**Proposition 2:** For all $\lambda \in \mathbb{R}$, the following exponential inequality holds

$$\mathbb{E}_{P_{U, z^m}, r_{1:N}} \left[ \exp \left( \lambda \tilde{\Delta} L(U, \hat{z}^m_{1:2N}, R, S_{1:N}) - \frac{\lambda^2 (b - a)^2}{2N} - I(U; R, S_{1:N}|\hat{z}^m_{1:2N}) \right) \right] \leq 1,$$  

(19)

where $P_{U, z^m, r_{1:N}} = P_{\hat{z}^m_{1:2N}, r_{1:N}} P_{U, z^m_{1:2N}, r_{1:N}}$ and $I(U; R, S_{1:N}|\hat{z}^m_{1:2N})$ is the following conditional information density:

$$I(U; R, S_{1:N}|\hat{z}^m_{1:2N}) = \log \frac{dP_{U, R, S_{1:N}}}{dP_{U, \hat{z}^m_{1:2N}, P_{R, S_{1:N}}}}.$$  

(20)

Using these inequalities, the proof of Theorem 1 can be completed as detailed in Appendix B.

**APPENDIX A**

**PROOF OF THEOREM 1**

Since $\ell(w, z)$ is bounded, we conclude that $\tilde{\Delta} L(w, y_{2N}, r, S_i)$ is bounded on $[a - b, b - a]$, and, hence, $\Delta L(w, y^N, r, S_i)$ is subgaussian with parameter $(b - a)/\sqrt{M}$ [16, Ex. 2.4]. Furthermore, since $\mathbb{E}_{P_{S_i} z^m_{(r, S_i)}}(W) = \mathbb{E}_{P_{S_i} z^m_{(r, S_i)}}(W)$, we have that $\mathbb{E}_{P_{S_i}}(\tilde{\Delta} L(w, y^N, r, S_i)) = 0$. Thus, we conclude that for every $w, y^N$, and $r_i$,

$$\mathbb{E}_{P_{S_i}} \left[ \exp \left( \lambda \tilde{\Delta} L(w, y^N, r, S_i) \right) \right] \leq \exp \left( \frac{\lambda^2 (b - a)^2}{2M} \right).$$  

(21)

Taking an additional expectation over $P_{W} z^m_{1:2N}, R_i$, we find that

$$\mathbb{E}_{P_{S_i} P_{W} z^m_{1:2N}, R_i} \left[ \exp \left( \lambda \left( \tilde{\Delta} L(W, \hat{z}^m_{1:2N}, R_i, S_i) - \frac{\lambda^2 (b - a)^2}{2M} \right) \right) \right] \leq 1.$$  

(22)

The desired result then follows from a change of measure from $P_{S_i} P_{W} z^m_{1:2N}, R_i$ to $P_{W} z^m_{1:2N}, S_i, R_i$ [15, Prop. 17.1(4)].

**APPENDIX B**

**PROOF OF THEOREM 1**

Substituting (15) into (14) and then (15) and (18) into (8), we conclude that

$$\mathbb{E}_{P_{U, z^m}, r_{1:N}} \left[ \tilde{\Delta} L(U, \hat{z}^m_{1:2N}, R, S_{1:N}) \right] = \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_{P_{U, z^m}, r_{1:N}} \left[ \tilde{\Delta} L(W, \hat{z}^m_{1:2N}, R_i, S_i) \right]$$  

$$+ \mathbb{E}_{P_{U, z^m}, r_{1:N}} \left[ \tilde{\Delta} L(U, \hat{z}^m_{1:2N}, R, S_{1:N}) \right].$$  

(23)

To bound the two terms on the right-hand side of (23), we use the exponential inequalities in Proposition 1 and 2. Specifically, applying Jensen’s inequality to (16) and (19), we find the following inequalities

$$\exp \left( \lambda \mathbb{E}_{P_{U, z^m}, r_{1:N}} \left[ \tilde{\Delta} L(W, \hat{z}^m_{1:2N}, R_i, S_i) \right] - \frac{\lambda^2 (b - a)^2}{2M} - I(W; S_i|\hat{z}^m_{1:2N}, R_i) \right) \leq 1,$$  

(24)

and

$$\exp \left( \lambda \mathbb{E}_{P_{U, z^m}, r_{1:N}} \left[ \tilde{\Delta} L(U, \hat{z}^m_{1:2N}, R, S_{1:N}) \right] - \frac{\lambda^2 (b - a)^2}{2N} - I(U; R, S_{1:N}|\hat{z}^m_{1:2N}) \right) \leq 1,$$  

(25)

where (24) and (25) are valid for every $\lambda \in \mathbb{R}$. Taking the log on both sides of the above inequalities, and optimizing over $\lambda$, we obtain upper bounds on the two expectations in (23) (similar to the one reported in [12, Cor. 5]), which, when substituted into (23), give the desired bound.

**REFERENCES**

[1] S. Shalev-Shwartz and S. Ben-David, *Understanding machine learning: From theory to algorithms*. Cambridge Univ. Press, 2014.

[2] J. Schmidhuber, “Evolutionary Principles in Self-Referential Learning, or On Learning How to Learn: The Meta-meta… Hook,” Ph.D. dissertation, Technische Universität München, 1987.

[3] S. Thrun and L. Pratt, “Learning to Learn: introduction and overview,” in *Learning to Learn*. Springer, 1998, pp. 3–17.

[4] J. Baxter, “A model of inductive bias learning,” Journal of Artif. Intell. Research, vol. 12, pp. 149–198, March 2000.

[5] D. Russo and J. Zou, “Controlling bias in adaptive data analysis using information theory,” in *Proc. Artif. Intell. Statist. (AISTATS)*, Cadiz, Spain, May 2016.

[6] A. Xu and M. Raginsky, “Information-theoretic analysis of generalization capability of learning algorithms,” in *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Long Beach, CA, USA, Dec. 2017.

[7] Y. Bu, S. Zou, and V. V. Veeravalli, “ Tightening mutual information based on generalization error,” in *Proc. IEEE Int. Symp. Inf. Theory (ISIT)*, Paris, France, July 2019.

[8] J. Negrea, M. Haghifam, G. K. Dziugaite, A. Khisti, and D. M. Roy, “Information-theoretic generalization bounds for SGLD via data-dependent estimates,” in *Proc. Conf. Neural Inf. Process. Syst. (NeurIPS)*, Vancouver, Canada, 2019.

[9] S. Thrun and L. Pratt, “Information-theoretic generalization bounds for SGLD via conditional mutual information,” 2020. [Online]. Available: https://arxiv.org/pdf/2005.04372.pdf

[10] Y. Steinke and L. Zakynthinou, “Reasoning about generalization via conditional mutual information,” arXiv, Feb. 2020. [Online]. Available: http://arxiv.org/abs/2001.09122
[11] A. Pentina and C. Lampert, “A PAC-bayesian bound for lifelong learning,” in International Conference on Machine Learning, 2014, pp. 991–999.

[12] J. Rothfuss, V. Fortuin, and A. Krause, “PACOH: Bayes-optimal meta-learning with PAC-guarantees,” arXiv preprint arXiv:2002.05551, 2020.

[13] R. Amit and R. Meir, “Meta-learning by adjusting priors based on extended PAC-bayes theory,” in International Conference on Machine Learning, 2018, pp. 205–214.

[14] F. Hellström and G. Durisi, “Generalization bounds via information density and conditional information density,” 2020. [Online]. Available: https://arxiv.org/abs/2005.08044v1

[15] Y. Polyanskiy and Y. Wu, Lecture notes on Information Theory, MIT (6.441), UIUC (ECE 563), Yale (STAT 664), 2019.

[16] M. Wainwright, High-Dimensional Statistics: A Non-Asymptotic Viewpoint. Cambridge, U.K: Cambridge Univ. Press, 2019.