AN ANALYSIS OF INFORMATION BOTTLENECKS

Anonymous authors
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ABSTRACT

Learning representations with information bottlenecks is a powerful information-theoretic approach for learning effective representations where unnecessary information is minimized while task-relevant information is maximized. Many machine learning algorithms have been derived based on information bottlenecks of representations. This study mathematically relates information bottlenecks of intermediate representations to the corresponding expected loss in general settings. We investigate the merit of our new mathematical findings with experiments across a range of architectures and learning settings. Through the theory and experiments, we provide a new foundation for understanding current and future methods for learning intermediate representations with information bottlenecks.

1 INTRODUCTION

The information bottleneck principle (Tishby et al., 1999; Slonim & Tishby, 2000) is an extension of the concept of minimal sufficient statistics for extracting information about target Y into representation Z from input X. It imposes an information bottleneck at representation Z by minimizing the mutual information between Z and X, $I(X;Z)$, while maximizing the mutual information between Z and Y, $I(Y;Z)$. Thus it defines a tradeoff between the complexity of representation Z and the sufficiency for predicting target Y. Imposing an information bottleneck by minimizing $I(X;Z)$ has been adopted in the machine learning literature as a common regularization technique (Alemi et al., 2016; 2018). When latent representations are stochastic, mutual information can be estimated by averaging log probabilities of latent representations over empirical samples; alternatively, tractable upper bounds can be computed (Kirsch et al., 2020; Kolchinsky & Tracey, 2017; Alemi et al., 2016). More generally, the notion of bottlenecks on representation expressivity has been used in work on structural inductive biases (Goyal & Bengio, 2022).

Consequently, understanding the connection between the information bottleneck regularizer $I(X;Z)$ and the generalization ability of machine learning models has become an active area of research. The previous work of Shwartz-Ziv et al. (2019) aimed to show that the gap between the expected loss and the training loss with n training data points can be bounded roughly (with high probability) by,

$$\tilde{\mathcal{O}}\left(\sqrt{\frac{2^{I(X;Z)}+1}{n}}\right) \quad \text{as } n \to \infty, \tag{1}$$

if the random variable Z is fixed and *not* learned from the training data that the training loss in the gap depends on. This result has been used to justify the information bottleneck principle in previous studies (Galloway et al., 2022).

While this bound is an important first step, it cannot be applied to end-to-end training of deep neural networks for two reasons. First, as pointed out by Hafez-Kolahi et al. (2020), the proof of this bound is incomplete, because it uses upper bounds as lower bounds and it ignores the effect of the input X outside of the information-theoretic *typical set*. Such effect is negligible sometimes in coding theory — one of the most classic and direct applications of information theory — but it is significant and not negligible in machine learning (Hafez-Kolahi et al., 2020). Second, and most importantly from the perspective of representation learning, the bound assumes that the latent random variable Z is fixed, and therefore does not take into account learning of the representation function. Indeed, if the representation function for Z is also learned from the same training data, the constraint on $I(X;Z)$ is fundamentally insufficient to guarantee generalization, as the representation function can overfit to training data even if $I(X;Z)$ is arbitrarily small (Hafez-Kolahi et al., 2020). Thus, the existing

theory fails to explain the success of the information bottleneck principle, which is typically used for learning intermediate representation functions in deep neural networks.

In this paper, we resolve this open question by providing novel and complete proofs for end-to-end learning of intermediate representations (Theorem 2) where the previous bound does not work. As a byproduct of our novel proofs, we also improve the previous bound significantly in the setting of the previous works with a fixed random variable Z (Theorem 1); i.e., we show that the gap between the expected loss and the training loss scales roughly (with high probability) as

$$\tilde{\mathcal{O}}\left(\sqrt{\frac{I(X;Z|Y)+1}{n}}\right) \quad \text{as } n \to \infty. \tag{2}$$

There are two significant improvements in our bound (2) when compared to the previous bound (1). First, we replace the exponential growth rate $2^{I(X;Z)}$ with the linear growth rate $I(X;Z)$. Second, we replace $I(X;Z)$ with $I(X;Z|Y)$, which is the expected mutual information between X and Z conditioned on Y. This is an improvement since $I(X;Z|Y) \leq I(X;Z)$ and we can decompose $I(X;Z)$ into two components by using the chain rule as (Federici et al., 2020):

$$I(X;Z) = I(X;Z|Y) + I(Y;Z). \tag{3}$$

Here, $I(X;Z|Y) \geq 0$ is the superfluous information that we want to minimize while maximizing the predictive information $I(Y;Z) \geq 0$. Therefore, regularizing $I(X;Z)$ while maximizing $I(Y;Z)$ is an indirect way to regularize $I(X;Z|Y)$. Accordingly, instead of regularizing $I(X;Z)$, recent works have considered regularizing $I(X;Z|Y)$ (Fischer, 2020; Federici et al., 2020; Lee et al., 2021). In terms of theory, replacing $I(X;Z)$ with $I(X;Z|Y)$ is qualitatively significant because $I(X;Z)$ cannot be zero while maintaining the label-relevant information $I(Y;Z)$, unlike $I(X;Z|Y)$.

Our main result (Theorem 2) shows that for end-to-end learning of intermediate representations, the gap between the expected loss and the training loss scales roughly (with high probability) as

$$\tilde{\mathcal{O}}\left(\min_{l\in\{1,2,\ldots,D+1\}}\sqrt{\frac{\mathbb{1}\{l\neq(D+1)\}I(X;Z_l^s|Y)+I(\phi_l^{\mathbf{S}};\mathbf{S})+1}{n}}\right) \quad \text{as } n\to\infty, \tag{4}$$

which reconciles representational complexity $I(X;Z_l^s|Y)$ with model complexity $I(\phi_l^{\mathbf{S}};\mathbf{S})$. Here, Z_l^s is the random variable of the l-th layer's representation with dependence on the given training dataset s, and D is the number of all layers, including the input layer and excluding the output layer; i.e., Z_1^s is the input layer, Z_D^s is the last hidden layer, and Z_{D+1}^s is the output layer. The value of the indicator function $\mathbb{1}\{l \neq (D+1)\}$ is one if $l \neq D+1$, and is zero if $l = D+1$. The term $I(\phi_l^{\mathbf{S}};\mathbf{S})$ measures the complexity of the representation model. These variables are defined in detail in Section 2.1. Our main contributions can be summarized as follows:

- In Section 3.1, we present the exponentially tighter sample complexity bound in the case of fixed representations.
- In Section 3.2, we present, to our knowledge, the first rigorous generalization bound for information bottleneck in the case of learning representations, showing that simplicity in both the representation and representation function are factors that support generalization.
- In Section 4, we conduct experiments to investigate our bounds and related generalization prediction metrics, finding that empirical estimates of the main factors in our bounds are strong predictors of the generalization gap.

For the setting of learning representations, our main contribution is *not* a tighter or computable generalization bound when compared to non-information-theoretic bounds (Vapnik, 1999; Bartlett & Mendelson, 2002). Instead, it is the new insight that the generalization gap is bounded with the information bottleneck regularizer $I(X;Z_l^s|Y)$ if we consider its tradeoff against the mutual information $I(\phi_l^{\mathbf{S}};\mathbf{S})$. This resolves the open question posed by a counter-example against generalization via information bottleneck in the previous work of Hafez-Kolahi et al. (2020), as explained below.

2 Preliminaries

We define the notation in Section 2.1 and discuss the direct previous results in Section 2.2.

2.1 Notation

We are given a training dataset $s = ((x_i, y_i))_{i=1}^n$ of n samples where $x_i \in \mathcal{X}$ and $y_i \in \mathcal{Y}$ are i.i.d. drawn from a joint distribution $\mathcal{P}$. We want to analyze the generalization gap, i.e., the gap between the expected loss and the training loss,

$$\mathbb{E}_{X,Y}[\ell(f^s(X),Y)] - \frac{1}{n}\sum_{i=1}^{n}\ell(f^s(x_i),y_i), \tag{5}$$

where $\ell : \mathbb{R}^{m_y} \times \mathcal{Y} \to \mathbb{R}_{\geq 0}$ is a bounded per-sample loss, and f^s represents a deep neural network learned with a given training dataset s. Here, X and Y are random variables for x and y with $(X,Y) \sim \mathcal{P}$. Similarly, we define $\mathbf{S}$ to be the random variable for the training dataset s. The separate notation of random variables and their instantiations is often used in the previous information-theoretic analyses (Xu & Raginsky, 2017; Shwartz-Ziv et al., 2019) and is important in our analyses to avoid ambiguities rigorously as we deal with separate sources of randomness. We use symbol $\circ$ to represent the composition of functions and the notation of $[D+1] = \{1, 2, \ldots, D+1\}$. We define the random variable of the output of the l-th layer by

$$Z_l^s = \phi_l^s \circ X, \tag{6}$$

where ϕ_l^s is the map for the first l layer with with $\phi_l^s(x) \in \mathcal{Z}_l^s$. That is, for any layer index $l \in [D+1]$, we can decompose the neural network f^s by

$$f^s = g_l^s \circ \phi_l^s, \tag{7}$$

where g_l^s is the map for the rest of the layers after l layers. For convenience, we refer to ϕ_l^s as the encoder and to g_l^s as the decoder, although it is unnecessary to have an explicit structure of an encoder and a decoder. Here, the case of $l = 1$ corresponds to the input layer where $\phi_1^s(x) = x$ and $g_1^s(x) = f^s(x)$. The case of $l = D+1$ corresponds to the output layer where $\phi_{D+1}^s(x) = f^s(x)$ and $g_{D+1}^s(q) = q$. We also decompose f^s by $f^s = h_{D+1}^s \circ h_D^s \circ h_{D-1}^s \circ \cdots \circ h_1^s$ where h_l^s represents the computation of the l-th layer; i.e., $\phi_l^s = h_l^s \circ h_{l-1}^s \circ \cdots \circ h_1^s$ and $g_l^s = h_{D+1}^s \circ h_D^s \circ \cdots \circ h_{l+1}^s$.

We denote by $\mathcal{A}$ the learning algorithm that returns the functions of each layer; i.e., $(h_l^s)_{l=1}^{D+1} = \mathcal{A}(s)$. Then, by taking a subset of the output coordinates, we define $\tilde{\mathcal{A}}_l(s) = (h_k^s)_{k=1}^{l}$. Finally, by composing the outputs of $\tilde{\mathcal{A}}_l$, we define $\mathcal{A}_l(s) = h_l^s \circ h_{l-1}^s \circ \cdots \circ h_1^s = \phi_l^s \in \mathcal{M}_l$. We then define the random variable of the encoder of the l-th layer by

$$\phi_l^{\mathbf{S}} = \mathcal{A}_l \circ \mathbf{S}. \tag{8}$$

Define the maximum loss $\mathcal{R}(f^s) = \sup_{(x,y)\in\mathcal{X}\times\mathcal{Y}} \ell(f^s(x),y)$. The direct previous work (Shwartz-Ziv et al., 2019) considers the realistic implementation on a computer (e.g., using floating point), which results in finite spaces for representations and models, i.e., $|\mathcal{Z}_l^s| < \infty$ and $|\mathcal{M}_l| < \infty$. We follow this setting while this can be easily discarded (see section 3.3 and appendix A.2).

2.2 Background

Hafez-Kolahi et al. (2020) noted that the previous work (Shwartz-Ziv et al., 2019) provided the following conjecture without complete mathematical proofs:

Conjecture 1. *(Shwartz-Ziv et al. (2019)) Let X be a d-dimensional random variable that obeys an ergodic Markov random field probability distribution asymptotically in d. Assume that $\mathbb{P}(X,Y)$ is bounded away from 0 and 1 (strictly inside the simplex interior). Then, for sufficiently large d, with probability at least $1-\delta$,*

$$\mathbb{E}_{X,Y}[\ell(f^s(X),Y)] - \frac{1}{n}\sum_{i=1}^{n}\ell(f^s(x_i),y_i) \leq \sqrt{\frac{2^{I(X;Z_l^s)} + \log\frac{2}{\delta}}{2n}} \tag{9}$$

In this conjecture, the encoder ϕ_l^s is fixed independently of training data s since the arguments of this conjecture implicitly assumes the independence of $Z_l^s = \phi_l^s \circ X$ and s. Indeed, the conjecture is proven to be false when the encoder ϕ_l^s is also learned with the training data s by a counter-example provided by Hafez-Kolahi et al. (2020). That is, as a straightforward example, one can consider the binary classification problem and an encoder $\phi_l^s(x_i) = y_i$ that is perfectly fitted to the training data s and compresses the information of X only to the information of 0 or 1. Then minimizing $I(X;Z_l^s)$ does not sufficiently constrain the complexity of ϕ_l^s, allowing it to arbitrarily overfit to the training data with a large generalization gap, in contradiction to the inequality (9). In other words, when selecting the encoder's parameters is part of the learning problem, measuring compression via $I(X;Z_l^s)$ does not capture the degree of overfitting of the encoder's parameters.

Accordingly, as a first step towards proving a sample complexity bound via information bottleneck, Hafez-Kolahi et al. (2020) focused on the input layer and proved the following input compression

bound for binary classification: if $\mathcal{Y} = \{0, 1\}$ and ℓ is the 0–1 loss, then for any $\delta > 0$, with probability at least $1 - \delta$, we have $\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(f^s(x_i), y_i) \leq \epsilon$, where ϵ is any fixed real number such that $\epsilon \geq \sqrt{18 \times \frac{2^{\frac{6H(X)}{\epsilon}} + \log\frac{1}{\delta} + 2}{n}}$, where where $H(X)$ is the entropy of X. If we ignore the factor $2^{\frac{1}{\epsilon}}$, this roughly concludes that

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(f^s(x_i), y_i) = \tilde{\mathcal{O}}\left(\sqrt{\frac{2^{H(X)}}{n}}\right). \tag{10}$$

Considering the factor $2^{\frac{1}{\epsilon}}$ only makes the bound worse (than eq. (10)) when the bound is non-vacuous; i.e., $\epsilon < 1$. It was discussed by the authors that generally the bound is loose due to domination of $2^{\frac{1}{\epsilon}}$ for small ϵ. The $\frac{1}{\epsilon}$ term appears despite the intuitive idea that $H(X)$ is the number of bits required to compress the signal X because $H(X)$ is the *expected* number of bits needed for transmitting a single sample without error. Establishing a high probability bound on the inference error requires controlling mass in the tail of the data distribution, introducing the term $\frac{1}{\epsilon}$.

Despite its popularity and its active usage in practice, there is no rigorous sample complexity bound for the information bottleneck principle, as noted by Hafez-Kolahi et al. (2020). Much of the work on information bottleneck assumes its benefits, as opposed to using sample complexity bounds to justify why it is desirable to control information bottlenecks. The present paper aims to fill this gap.

3 Analysis

In this section, we establish sample complexities for information bottlenecks. We begin in Section 3.1 with the setting of previous papers (Shwartz-Ziv et al., 2019; Hafez-Kolahi et al., 2020), where the encoder ϕ_l^s is fixed independently of training data s. Then we extend this result to the setting of learning the encoder ϕ_l^s with s in Section 3.2, which is the main theoretical result of this paper.

3.1 Fixed Encoder

The following theorem shows that we can indeed minimize the expected loss by minimizing the conditional mutual information $I(X; Z_l^s|Y)$ and the training loss if the encoder ϕ_l^s is fixed:

Theorem 1. *Let $l \in \{1, \dots, D\}$. Suppose that ϕ_l^s is fixed independently of the training dataset s. Then, for any $\gamma_l > 0$ and $\delta > 0$, with probability at least $1 - \delta$, the following holds:*

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(f^s(x_i), y_i) \leq G_3^l \sqrt{\frac{I(X; Z_l^s|Y)\ln(2) + \mathcal{G}_2^l}{n}} + \frac{G_1^l(0)}{\sqrt{n}}, \tag{11}$$

where $G_1^l(0) = \tilde{\mathcal{O}}(1)$, $\mathcal{G}_2^l = \tilde{\mathcal{O}}(1)$, and $G_3^l = \tilde{\mathcal{O}}(1)$, as $n \to \infty$. Moreover, the formula of $G_1^l(0)$, $\mathcal{G}_2^l$ and G_3^l are given in appendix A.1.

Theorem 1 rigorously completes the proof of Conjecture 1, with the significant improvements by reducing the exponential dependence to the linear dependence, and by replacing the mutual information with the conditional mutual information. Theorem 1 is applicable when the encoder is learned with data independent of s: e.g., some cases in transfer learning and unsupervised learning.

3.2 Encoder Learned with the Same Training Data

In the previous section, we have proven an improved version of Conjecture 1 for the setting with a fixed encoder ϕ_l^s where the conjecture is possibly valid. However, the typical usage of the information bottleneck principle is approximately minimizing $I(X; Z_l^s) = I(X; \phi_l^s \circ X)$ over the parameters of the encoder ϕ_l^s, in conjunction with a discriminative objective. Thus, to support the typical usage of the principle, we need to extend the results to the setting of learning encoder ϕ_l^s with s. In this setting, the bound in Conjecture 1 is false as discussed in Section 2.2. Thus, natural open questions are the following: can we prove a sample complexity bound with the information bottleneck in this setting? If we can, what are the appropriate bounds?

We now present our main theorem that answers these questions by providing the sample complexity bound, which reconciles the information bottleneck regularizer $I(X; Z_l^s|Y)$ with the mutual information of the encoder and the training dataset $I(\phi_l^{\mathbf{S}}; \mathbf{S})$:

Theorem 2. *Let $\mathcal{D} \subseteq \{1, 2, \dots, D+1\}$, $\gamma_l > 0$ and $\lambda_l > 0$ for all $l \in \mathcal{D}$. Then, for any $\delta > 0$, with probability at least $1-\delta$, the following holds:*

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(f^s(x_i), y_i) \leq \min_{l \in \mathcal{D}} Q_l, \tag{12}$$

$$\text{where } Q_l = \begin{cases} G_3^l \sqrt{\frac{\left(I(X;Z_l^s|Y) + I(\phi_l^{\mathbf{S}};\mathbf{S})\right)\ln(2) + \widehat{\mathcal{G}}_2^l}{n}} + \frac{G_1^l(\zeta)}{\sqrt{n}} & \text{if } l \leq D \\ \mathcal{R}(f^s)\sqrt{\frac{I(\phi_l^{\mathbf{S}};\mathbf{S})\ln(2) + \check{\mathcal{G}}_2^l}{2n}} & \text{if } l = D+1, \end{cases}$$

with $G_1^l(\zeta) = \tilde{\mathcal{O}}(\sqrt{I(\phi_l^{\mathbf{S}};\mathbf{S}) + 1})$, $\widehat{\mathcal{G}}_2^l = \tilde{\mathcal{O}}(1)$, $\check{\mathcal{G}}_2^l = \tilde{\mathcal{O}}(1)$, and $G_3^l = \tilde{\mathcal{O}}(1)$ as $n \to \infty$. Moreover, the formulas of $G_1^l(\zeta)$, $\widehat{\mathcal{G}}_2^l$, $\check{\mathcal{G}}_2^l$, and G_3^l are given in appendix A.1.

The main factor $I(X; Z_l^s|Y) + I(\phi_l^{\mathbf{S}}; \mathbf{S})$ in Theorem 2 makes sense and captures the novel tradeoff that has not been studied in any previous sample complexity bounds. That is, this captures the tradeoff between "how much information from the input X the trained encoder ϕ_l^s retains (i.e., $I(X; Z_l^s|Y)$)" v.s. "how much information from the training dataset $\mathbf{S}$ is used to train the encoder $\phi_l^{\mathbf{S}}$ (i.e., $I(\phi_l^{\mathbf{S}}; \mathbf{S})$)". Theorem 2 is applicable when the encoder is trained with s and potentially additional data independent of s: e.g., supervised learning, semi-supervised learning, unsupervised learning, and transfer learning. For example, Theorem 2 captures the benefit of transfer learning in both terms of $I(X; Z_l^s|Y)$ and $I(\phi_l^{\mathbf{S}}; \mathbf{S})$ since the encoder $\phi_l^{\mathbf{S}}$ is expected to have less dependence on the target data $\mathbf{S}$ (for some $l \leq D$) in transfer learning, which tends to decrease $I(\phi_l^{\mathbf{S}}; \mathbf{S})$. Here, $I(\phi_l^{\mathbf{S}}; \mathbf{S})$ is measuring the effect of overfitting the encoder, which is necessary to avoid the counter-example (Hafez-Kolahi et al., 2020, Example 3.1).

Therefore, Theorem 2 provides the first rigorous sample complexity bound for the information bottleneck in the setting of training the encoder $\phi_l^{\mathbf{S}}$ with the same training data s. A related yet different topic of information theory uses $I(f^{\mathbf{S}}; \mathbf{S})$ to compute sample complexity bounds (Xu & Raginsky, 2017; Bassily et al., 2018). These previous bounds are *not* about information bottleneck as these do *not* utilize $I(X; Z_l^s|Y)$ (or $I(X; Z_l^s)$) and only uses $I(f^{\mathbf{S}}; \mathbf{S})$, the mutual information between the training dataset $\mathbf{S}$ and the *entire* model $f^{\mathbf{S}} = \phi_{D+1}^{\mathbf{S}}$. Thus, the previous bounds cannot provide insights or justifications on the information bottleneck principle unlike our bounds. Moreover, in Section 4, we demonstrate the advantage of $I(X; Z_l^s|Y) + I(\phi_l^{\mathbf{S}}; \mathbf{S})$ in our bound over $I(f^{\mathbf{S}}; \mathbf{S})$ in the previous bounds. Here, notice that $I(\phi_l^{\mathbf{S}}; \mathbf{S}) \neq I(f^{\mathbf{S}}; \mathbf{S})$ for any $l \neq D+1$, and $I(\phi_1^{\mathbf{S}}; \mathbf{S}) \leq \cdots \leq I(\phi_D^{\mathbf{S}}; \mathbf{S}) \leq I(\phi_{D+1}^{\mathbf{S}}; \mathbf{S}) = I(f^{\mathbf{S}}; \mathbf{S})$ always (e.g., see Figure 2). See appendix A.3 for more discussions about the previous bounds, which is *not* of information bottleneck.

Let us consider the parameterization of the encoder as $\phi_l^{\mathbf{S}} = \phi_{l,\theta_l^{\mathbf{S}}}$ where $\theta_l^{\mathbf{S}}$ is the parameter vector that is learned with $\mathbf{S}$ and contains all parameters of the layers up to l-th layer:

Remark 1. Theorem 2 holds when replacing $\phi_l^{\mathbf{S}}$ with $\theta_l^{\mathbf{S}}$.

Finally, the following proposition shows that deterministic neural networks with continuous distributions can have finite mutual information with ReLU activations:

Proposition 1. *If we use ReLU activations, then there are infinitely many continuous distributions over $\mathcal{X}$ such that there are deterministic neural networks with finite $I(X, Z|Y)$.*

3.3 Application to The Case of Infinite Mutual Information

The mutual information for the information bottleneck is finite for many practical cases including the cases of discrete domains $\mathcal{X}$ with any models and of continuous domains $\mathcal{X}$ with stochastic models as well as the case in Proposition 1 with ReLU. Therefore, there is no problem with discrete domain input, stochastic networks and ReLU networks. However, it is infinite for some special case, for example, of continuous domains $\mathcal{X}$ with deterministic neural networks with certain types of injective activations such as sigmoid (instead of ReLU) (Amjad & Geiger, 2019). This subsection demonstrates that our bounds produces finite bounds even for any special cases of the mutual information being infinite. Our results (Theorems 1–2 with Corollary 1) also resolve the known issue of arbitrariness of the mutual information with different binning methods (Saxe et al., 2019).

Consider an arbitrary (continuous or discrete) domain $\mathcal{X}$ and an arbitrary encoder $\tilde{\phi}_l^s$ such that $\tilde{\phi}_l^s(x) \in \tilde{\mathcal{Z}}_l^s$ and the set $\tilde{\mathcal{Z}}_l^s$ is potentially (uncountably or countably) infinite. Define the corre-

sponding model $\tilde{f}^s$ by $\tilde{f}^s = g_l^s \circ \tilde{\phi}_l^s$ and $\tilde{Z}_l^s = \tilde{\phi}_l^s \circ X$. We formalize an arbitrary binning method $\mathcal{E}_l[\tilde{\phi}_l^s]$ of computing the mutual information (Chelombiev et al., 2019) as follows: for any $(l, \tilde{\phi}_l^s)$, let $\mathcal{E}_l[\tilde{\phi}_l^s] : \tilde{\mathcal{Z}}_l^s \to \mathcal{Z}_l^s \subseteq \tilde{\mathcal{Z}}_l^s$ be a function such that $|\mathcal{Z}_l^s| < \infty$. Set $\phi_l^s = \mathcal{E}_l[\tilde{\phi}_l^s] \circ \tilde{\phi}_l^s$; i.e., it follows that $Z_l^s = \mathcal{E}_l[\tilde{\phi}_l^s] \circ \tilde{Z}_l^s$ and $f^s = g_l^s \circ \mathcal{E}_l[\tilde{\phi}_l^s] \circ \tilde{\phi}_l^s$. Let $\hat{Q}_l$ and $\min_{l \in \mathcal{D}} Q_l$ be the right-hand side of eq. (11) and eq. (12) in Theorems 1–2 with this choice of encoder ϕ_l^s; i.e., $\hat{Q}_l$ and Q_l contain $I(X; Z_l^s|Y)$ instead of $I(X; \tilde{Z}_l^s|Y)$. Here, $I(X; Z_l^s|Y)$ is the mutual information computed by the binning method $\mathcal{E}_l[\tilde{\phi}_l^s]$ while $I(X; \tilde{Z}_l^s|Y)$ is the true mutual information of $\tilde{f}^s$. Let C_l be a nonnegative real number such that $\mathbb{P}(|\ell((g_l^s \circ \tilde{\phi}_l^s)(X), Y) - \ell((g_l^s \circ \mathcal{E}_l[\tilde{\phi}_l^s] \circ \tilde{\phi}_l^s)(X), Y)| \leq C_l) = 1$.

Corollary 1 shows that even when the mutual information $I(X; \tilde{Z}_l^s|Y)$ of the original model $\tilde{f}^s$ is infinite, Theorems 1–2 provide the finite bounds on the *original* model $\tilde{f}^s$ using the finite mutual information $I(X; Z_l^s|Y)$ returned by a binning method $\mathcal{E}_l[\tilde{\phi}_l^s]$:

Corollary 1. *Suppose that $C_l < \infty$. Then, Theorems 1–2 hold true also when we replace*
(Theorem 1) *eq.* (11) *with* $\mathbb{E}_{X,Y}[\ell(\tilde{f}^s(X), Y)] - \frac{1}{n}\sum_{i=1}^n \ell(\tilde{f}^s(x_i), y_i) \leq \hat{Q}_l + 2C_l < \infty$, *and,*
(Theorem 2) *eq.* (12) *with* $\mathbb{E}_{X,Y}[\ell(\tilde{f}^s(X), Y)] - \frac{1}{n}\sum_{i=1}^n \ell(\tilde{f}^s(x_i), y_i) \leq \min_{l \in \mathcal{D}} Q_l + 2C_l < \infty$.

The assumption on the finiteness of C_l is satisfied for common scenarios. For example, let L be the Lipschitz constant of the function $q \mapsto \ell(g_l^s(q), Y)$ w.r.t. some metric $d_{\mathcal{E}}$ almost surely (Fazlyab et al., 2019; Latorre et al., 2019; Aziznejad et al., 2020; Pauli et al., 2021). Set $\mathcal{E}_l[\tilde{\phi}_l^s]$ such that the radius of each bin w.r.t. the metric $d_{\mathcal{E}}$ is at most $\epsilon/\sqrt{nL^2}$ for some $\epsilon > 0$. We can then set

$$C_l = \frac{\epsilon}{\sqrt{n}}. \tag{13}$$

In Corollary 1, the arbitrariness with binning methods is resolved: e.g., increasing the bin size ϵ can decrease the mutual information, but it also increases the value of $C_l = \frac{\epsilon}{\sqrt{n}}$. Thus, there is always a tradeoff and we cannot arbitrarily change values of our bounds by choosing different binning methods. Similarly, for the case of infinite mutual information, we prove the validity of general methods of computing mutual information, including those of injecting noises and kernel density estimations, in appendix A.2.

3.4 Proof Sketch

This subsection provides proof sketches for Theorems 1-2. The full proofs of Theorems 1-2, Corollary 1, and Remark 1 are completed in appendix B.

Proof Sketch of Theorem 1. Fix $l \in [D]$ and ϕ_l^s independently of the training dataset s. Let T be the standard typical set of Z_l^s of information theory. We first decompose the generalization gap into two terms as $\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^n \ell(f^s(x_i), y_i) = A + B$, where A corresponds to the case of $Z_l^s \in T$, while B is for the case of $Z_l^s \notin T$. Using the standard argument from information theory, we have $\mathbb{P}(Z_l^s \notin T \mid Y = y) \leq \mathcal{O}(1/\sqrt{n})$ (where the probability is with respect to X), with which we can almost argue that $B \leq \mathcal{O}(1/\sqrt{n})$ although this requires a refinement of the standard argument. In appendix B, we refine the argument using the McDiarmid's inequality and a further decomposition of B. To bound A, we argue that A is bounded by a concentration gap of a special multinomial distribution over the elements of T, which is bounded roughly as $A = \mathcal{O}(\sqrt{(\ln |T|)/n})$ (with high probability with respect to $\mathbf{S}$), by using a recent statistical result on multinomial distributions (Kawaguchi et al., 2022, Lemma 3 & Proposition 3). Then, the standard argument from information theory approximately bounds the size of the typical set as $|T| \leq 2^{I(X;Z_l^s|Y)+C_T}$ for some $C_T > 0$, roughly resulting in $A = \mathcal{O}(\sqrt{(\ln |T|)/n}) = \tilde{\mathcal{O}}(\sqrt{(I(X; Z_l^s|Y) + 1)/n})$ (with high probability). By combining these bounds on A and B, we approximately conclude that $\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^n \ell(f^s(x_i), y_i) = A + B = \tilde{\mathcal{O}}(\sqrt{(I(X; Z_l^s|Y) + 1)/n})$ (with high probability). As can be seen in this sketch, we combine deterministic decompositions and probabilistic bounds with respect to the randomness of new fresh samples X and datasets $\mathbf{S}$. The usages of probabilistic bounds for different sample spaces enable the exponential improvement over the previous bounds. The full proof of Theorem 1 is presented in appendix B. □

Proof Sketch of Theorem 2. We reuse the result of Theorem 1 for fixed $l \in [D]$ and ϕ_l^s, and we generalize it for flexible l and learnable ϕ_l^s. The careful usage of probabilistic bounds for different

sample spaces in the proof of Theorem 1 enables the proof for the setting of learning encoder. Let $l \in [D]$. We first find a hypothesis space Φ_δ^l such that $\mathbb{P}(\phi_l^{\mathbf{S}} \notin \Phi_\delta^l) \leq \delta$ and $|\Phi_\delta^l| \leq 2^{I(\phi_l^{\mathbf{S}};\mathbf{S})+C_\delta}$ for some $C_\delta \geq 0$. We then construct the corresponding hypothesis space $\mathcal{H}$ by $\mathcal{H} = \cup_{\phi_l \in \Phi_\delta^l} \mathcal{H}_{\phi_l}$ where $\mathcal{H}_{\phi_l} = \{g_l \circ \phi_l \mid g_l : \mathcal{Z}_l \to \mathbb{R}^{m_y}\}$. We now obtain the sample complexity bound for each $\mathcal{H}_{\phi_l}$ (for each $\phi_l \in \Phi_\delta^l$) by using the result of Theorem 1 for each $\phi_l \in \Phi_\delta^l$ that is fixed independently of s; i.e., $\mathbb{P}(\forall f \in \mathcal{H}_{\phi_l}, \mathcal{B}(f) \leq J_l(\delta)) \geq 1-\delta$ where $\mathcal{B}(f) = \mathbb{E}_{X,Y}[\ell(f(X),Y)] - \frac{1}{n}\sum_{i=1}^n \ell(f(x_i),y_i)$ and $J_l(\delta)$ is the right-hand side of eq. (11). Then, by taking union bound with the equal weighting over all $\phi_l \in \Phi_\delta^l$, we have $\mathbb{P}(\forall f \in \mathcal{H}, \mathcal{B}(f) \leq J_{\delta,l}) \geq 1-\delta$ where $J_{\delta,l} = J_l(\delta/(2^{I(\phi_l^{\mathbf{S}};\mathbf{S})+C_\delta}))$. We now want to show that this bound holds for $\mathcal{B}(f^s)$ instead of $\mathcal{B}(f)$ for $f \in \mathcal{H}$. This is achieved if $f^s \in \mathcal{H}$. Since $\mathbb{P}(f^{\mathbf{S}} \in \mathcal{H}) \geq 1-\delta$ from the construction of $\mathcal{H}$ and $\mathbb{P}(A \cap B) \leq \mathbb{P}(B)$ for any events A and B, the following holds:

$$\begin{aligned}\mathbb{P}(\mathcal{B}(f^{\mathbf{S}}) \leq J_{\delta,l}) \geq \mathbb{P}(f^{\mathbf{S}} \in \mathcal{H} \bigcap \mathcal{B}(f^{\mathbf{S}}) \leq J_{\delta,l}) &= \mathbb{P}(f^{\mathbf{S}} \in \mathcal{H})\mathbb{P}(\mathcal{B}(f^{\mathbf{S}}) \leq J_{\delta,l} \mid f^{\mathbf{S}} \in \mathcal{H}) \\ &\geq \mathbb{P}(f^{\mathbf{S}} \in \mathcal{H})(1-\delta) \geq 1-2\delta.\end{aligned}$$

Therefore, by replacing δ with $\delta/2$, we have $\mathbb{P}(\mathcal{B}(f^{\mathbf{S}}) \leq J_{\delta/2,l}) \geq 1-\delta$. For the case of $l = D+1$, the proof is significantly simplified because an entire model is an encoder as $f = \phi_{D+1}$; i.e., we replace the result of Theorem 1 with Hoeffding's inequality to conclude that $\mathbb{P}(\forall f \in \mathcal{H}_{\phi_{D+1}}, \mathcal{B}(f) \leq J_{D+1}(\delta)) \geq 1-\delta$ where $J_{D+1}(\delta) = \mathcal{R}(f)\sqrt{(\ln(1/\delta))/(2n)}$. Using the same steps as the case of $l \in [D]$, we prove that $\mathbb{P}(\mathcal{B}(f^{\mathbf{S}}) \leq J_{\delta/2,D+1}) \geq 1-\delta$, where $J_{\delta,D+1} = J_{D+1}(\delta/(2^{I(\phi_l^{\mathbf{S}};\mathbf{S})+C_\delta}))$. By taking union bounds over $l \in \mathcal{D} \subseteq \{1,2,\ldots,D+1\}$, we conclude $\mathbb{P}(\forall l \in \mathcal{D}, \mathcal{B}(f^{\mathbf{S}}) \leq J_{\delta/(2|\mathcal{D}|),l}) = \mathbb{P}(\mathcal{B}(f^{\mathbf{S}}) \leq \min_{l\in\mathcal{D}} J_{\delta/(2|\mathcal{D}|),l}) \geq 1-\delta$. Finally, organizing the expression of $J_{\delta/(2|\mathcal{D}|),l}$ yields the right-hand side of eq. (12), which proves Theorem 2. The full proof of Theorem 2 is presented in appendix B. □

4 Experiments

We conduct empirical experiments to investigate the following questions:

- Does the information bottleneck regularizer $I(X;Z_l^s)$ alone reliably predict generalization when the encoder ϕ_l^s is learned with s?
- Does the main factor $\min_{l\in[D]} I(\mathbf{S};\theta_l^{\mathbf{S}}) + I(X;Z_l^s|Y)$ in Theorem 2 with Remark 1 predict generalization more accurately than $I(X;Z_l^s)$ alone (or $I(X;Z_l^s|Y)$ alone)?
- How does varying layer l within the network affect the values of $I(\mathbf{S};\theta_l^{\mathbf{S}})$ and $I(X;Z_l^s)$ and their predictive ability?

4.1 On the Representation Compression Bound

As discussed in Sections 3 and 2, $I(X;Z_l^s)$ is generally not a reliable predictor of generalization because feature compression does not prevent the overfitting of the representation function's parameters. We investigate this further by designing a learning algorithm that trains models under various hyperparameter settings with the constraint that estimated $I(X;Z_l^s)$ is approximately constant.

The inference problem studied was 5 class classification on clustered 2D inputs (fig. 3). The model architecture was a 5 layer MLP with deterministic weights and feature layer l was fixed to the penultimate layer. Given training dataset s, each model q_θ was optimized with the cross-entropy loss $\text{minimize}_\theta -(1/|s|)\sum_{(x,y)\in s}(\log(1/k)\sum_{j=1}^k q_\theta(y|z^j))$ s.t. $\hat{I}(X;Z_l^s) = \rho$, where features $z^j \sim q_\theta(Z_l^s|x)$, $q_\theta(Z_l^s|x)$ is a multivariate Normal distribution with mean and variance computed by the MLP, $\hat{I}(X;Z_l^s) = (1/|s|)\sum_{(x,y)\in s}(1/k)\sum_{j=1}^k \log(q_\theta(z^j|x)/((1/|s|)\sum_{(x',y')\in s} q_\theta(z^j|x')))$ is a Monte-Carlo sampling based estimator of $I(X;Z_l^s)$, and constraint ρ was set to 1.5, approximately half the value of $\hat{I}(X;Z_l^s)$ attained without constraining $\hat{I}(X;Z_l^s)$. The neural network infers a distribution over a stochastic latent features so that $\hat{I}(X;Z_l^s)$ can be regularized and evaluated directly during training; in section 4.2 we consider the case of deterministic features without regularization of $\hat{I}(X;Z_l^s)$. The learning algorithm is defined by the posterior distribution over network parameters $\mathbb{P}(\theta_l^{\mathbf{S}}|\mathbf{S}=s)$, which was modelled using SWAG (Maddox et al., 2019; Mandt et al., 2017), chosen for its popularity and simplicity. We denote the estimator of $I(\mathbf{S};\theta_l^{\mathbf{S}})$ using SWAG by $\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})$ (appendix C). To account for different scales of different estimation procedures, we tested rescaling $\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})$ by the average value of $\hat{I}(X;Z_l^s|Y)$, denoting rescaled values by $\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}})$ (appendix C).

	Pearson c.		Pearson c.
Num. params.	- 0.0294	$\breve{I}(\mathbf{S};\theta^{\mathbf{S}}_{D+1})$	0.0091
$\prod_{\mathbf{l}}\|\theta^{\mathbf{S}}_{\mathbf{l}}\|_F$	-0.0871	$\breve{I}(\mathbf{S};\theta^{\mathbf{S}}_{l})$	0.0211
$\breve{I}(X;Z^s_l)$	0.3712	$\tilde{I}(\mathbf{S};\theta^{\mathbf{S}}_{l}) + \breve{I}(X;Z^s_l)$	**0.3928**
$\breve{I}(X;Z^s_l\|Y)$	0.3842	$\tilde{I}(\mathbf{S};\theta^{\mathbf{S}}_{l}) + \breve{I}(X;Z^s_l\|Y)$	**0.4130**

Table 1: Pearson correlation coefficient between metrics and the generalization gap in loss for constrained models. Positive values denote positive correlations. $\theta^{\mathbf{S}}_{\mathbf{l}}$ denotes parameters of layer $\mathbf{l}$ and $\theta^{\mathbf{S}}_{l}$ denotes parameters up to layer l.

216 models were trained over varying architectures, weight decay rates, dataset draws, and random seeds. Model parameters were optimized end-to-end using the reparameterization trick (Kingma et al., 2015) with dual gradient descent (Bertsekas, 2014). See appendix C for more details on the experimental setup. For each model, we measured the generalization gap between the test set and train set losses. We found that combining model compression and representation compression yielded the best predictor of generalization overall, and that this outperformed using representation compression alone (tables 1 and 5). We additionally report results for MNIST and Fashion MNIST datasets and small convolutional networks (appendix D), empirically finding that this conclusion also holds for stochastic latent representation models when $I(X;Z^s_l)$ is unconstrained.

4.2 Image Classification

To investigate a common setting, we tested the metrics on image classification models with larger architectures and standard cross-entropy training without explicitly constraining any mutual information (MI). We trained 540 deep neural networks on CIFAR10, over varying preactivation ResNet architectures (He et al., 2016), weight decay rates, batch sizes, dataset draws and random seeds.

To study representation compression by estimating MI with deterministically computed features, noise is customarily injected purely for analysis purposes (Saxe et al., 2019). We tested adaptive kernel density estimation (KDE) (Chelombiev et al., 2019), which models the latent represenation of an input as a unimodal Gaussian centred at the deterministic feature, with variance σ^2_l determined by scaling a base value according to maximum observed activation value in the layer. We also tested selecting σ^2_l by maximum likelihood estimation (MLE) of observed features under the constraint that estimated MI decreases with layer, which follows from the information processing inequality. We report the results in this section for MLE and in appendix E.4 for adaptive KDE. Representations were taken from $D = 5$ layers in the model, ranging from the input to the output of the penultimate layer. Again, SWAG was used to model the posterior $\mathbb{P}(\theta^{\mathbf{S}}_l|\mathbf{S} = s)$ for computing $\breve{I}(\mathbf{S};\theta^{\mathbf{S}}_l)$. Since SWAG approximates the stationary distribution of SGD from a fixed initialization as a unimodal Gaussian (Mandt et al., 2017), we also tested averaging over initializations to obtain a richer posterior model, and denote the estimator of MI from this model as $\bar{I}(\mathbf{S};\theta^{\mathbf{S}}_l)$, defined in appendix E.2. To construct multiple instances of the training dataset, we sampled 5 training sets of size 15K from the CIFAR10 training set, and each test set was the original 10K test set.

We found that the generalization gap was positively correlated with metrics measuring representation compression, but even more correlated with metrics that combined both representation and model compression (table 2). By increasing the value of layer index l of the encoder, MI between the encoder and

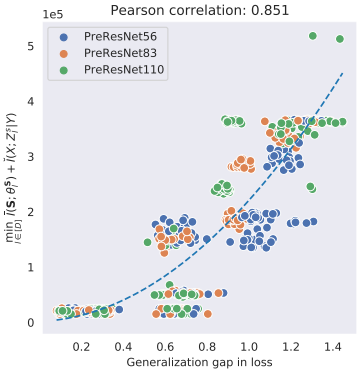

Figure 1: Results for $\min_{l\in[D]} \bar{I}(\mathbf{S};\theta^{\mathbf{S}}_l) + \breve{I}(X;Z^s_l|Y)$ for unconstrained models trained on CIFAR10. Dashed line denotes best polynomial fit with degree 2.

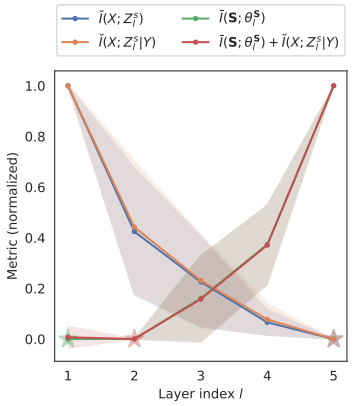

Figure 2: Metrics averaged over models for each layer index. Values are normalized by subtracting the minimum and dividing by the range. Star denotes minimum.

Generalization gap:	Spearman corr. Loss	Spearman corr. Error	Pearson corr. Loss	Pearson corr. Error	Kendall corr. Loss	Kendall corr. Error
$\frac{1}{D}\sum_{l=1}^{D}\breve{I}(X;Z_l^s)$	0.8481	0.7410	0.2116	0.1831	0.6425	0.5436
$\min_{l\in[D]}\breve{I}(X;Z_l^s)$	0.7145	0.5602	0.7203	0.5719	0.4461	0.3404
$\frac{1}{D}\sum_{l=1}^{D}\breve{I}(X;Z_l^s\|Y)$	0.8481	0.7406	0.2140	0.1853	0.6427	0.5435
$\min_{l\in[D]}\breve{I}(X;Z_l^s\|Y)$	0.7004	0.5434	0.7062	0.5560	0.4386	0.3305
$\breve{I}(\mathbf{S};\theta_{D+1}^{\mathbf{S}})$	0.4688	0.3112	0.2512	0.0775	0.2121	0.1208
$\min_{l\in[D]}\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s\|Y)$	0.8434	0.7313	0.8437	0.7195	0.6270	0.5332
$\bar{I}(\mathbf{S};\theta_{D+1}^{\mathbf{S}})$	0.5370	0.3800	0.2924	0.1218	0.2442	0.1526
$\min_{l\in[D]}\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s\|Y)$	**0.8632**	**0.7576**	**0.8511**	**0.7562**	**0.6626**	**0.5664**

Table 2: Correlation results across metrics for CIFAR10 models. Each value is in [-1, 1] and > 0 indicates positive correlation. Best metric highlighted. More results can be found in appendix E.

Generalization gap:	Spearman corr. Loss	Spearman corr. Error	Pearson corr. Loss	Pearson corr. Error	Kendall corr. Loss	Kendall corr. Error
$\frac{1}{D}\sum_{l=1}^{D}\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s\|Y)$	0.4429	0.2908	0.2783	0.1059	0.2349	0.1426
$\max_{l\in[D]}\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s\|Y)$	0.5711	0.4204	0.2993	0.1311	0.2886	0.1945
$\min_{l\in[D]}\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s\|Y)$	**0.8632**	**0.7576**	**0.8511**	**0.7562**	**0.6626**	**0.5664**
$\bar{I}(\mathbf{S};\theta_1^{\mathbf{S}})+\breve{I}(X;Z_1^s\|Y)$	0.6476	0.5292	0.1557	0.1331	0.4307	0.3504
$\bar{I}(\mathbf{S};\theta_D^{\mathbf{S}})+\breve{I}(X;Z_D^s\|Y)$	0.5711	0.4204	0.2993	0.1311	0.2886	0.1945

Table 3: Correlation results for $\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s|Y)$ for CIFAR10 models across different layer summarization methods.

training dataset increased, while MI between the representation and input decreased (fig. 2), capturing a trade-off between these two measures of compression.

Empirically, metrics of representation compression based on Monte-Carlo sampling ($\hat{I}(X;Z_l^s)$) and the upper bound ($\breve{I}(X;Z_l^s)$) were both strongly correlated with the generalization gap, with the latter outperforming the former (table 17), while for model compression, $\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})$ demonstrated higher correlation than $\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})$ (table 2). For selection of hyperparameters σ_l^2, MLE (figs. 1 and 2 and tables 2, 3, 15 and 17) outperformed adaptive KDE (tables 16 and 18). However, regardless of which scheme was used, the best metric that combined representation compression and model compression outperformed the best metric for representation compression or model compression individually. $\min_{l\in[D]}\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s|Y)$ was the strongest metric overall and is illustrated in fig. 1. Taking the minimum over layers (theorem 2) outperformed other layer summarization methods (table 3). The experiments indicate that metrics which combine model compression with representation compression are better predictors of generalization than measures of either representation compression or model compression alone.

5 Conclusion

This study first completed the proof of the previous conjecture with near-exponential improvements for the setting of fixed representations, then proved the first rigorous generalization bound for the setting of learning representations, and further strengthened the new findings with experiments. This paper does not make any claim on whether information bottlenecks can explain well the performance of current deep neural networks without information bottleneck methods, which is studied in a related yet different subfield (Shwartz-Ziv & Tishby, 2017; Saxe et al., 2019). Instead, the focus of this paper is on the technical contributions relevant for current and future methods of learning representations with information bottlenecks. Another related yet different topic focuses on deriving bounds on the difference between the mutual information $I(X;Z_l^s)$ and its empirical estimator (Shamir et al., 2010; Vera et al., 2018), which can be combined with our results.

REPRODUCIBILITY STATEMENT

For the theoretical results, complete proofs are provided. For the empirical experiments, source code is provided with the supplementary material.

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A ADDITIONAL RESULTS AND EXPLANATIONS FOR THEORY

We present additional results and explanations for theoretical results in appendix A, full proofs in appendix B, and additional results and details for experimental results in appendix C.

A.1 ON THEOREMS 1–2

The mutual information $I(\phi_l^{\mathbf{S}}; \mathbf{S})$ in Theorem 2 does not appear in Conjecture 1. However, the sample complexity bound in Conjecture 1 is invalid for the setting of learning ϕ_l^s, because the encoder ϕ_l^s can overfit to the training data, which was demonstrated with the counter-example in Hafez-Kolahi et al. (2020, Example 3.1). The mutual information $I(\phi_l^{\mathbf{S}}; \mathbf{S})$ is measuring the effect of overfitting the encoder, which is necessary to avoid the counter-example.

Using additional notation defined in appendix A.1.1, we will discuss the details of the formulas of $G_1^l(0)$, $\mathcal{G}_2^l$ and G_3^l of Theorems 1 and $G_1^l(\zeta)$, $\widehat{\mathcal{G}}_2^l$, $\check{\mathcal{G}}_2^l$, and G_3^l of Theorem 2 in appendix A.1.2.

A.1.1 ADDITIONAL NOTATION

We define the variables for the (hidden) input generating process as follows. Each $x \in \mathcal{X}$ is generated with a hidden function χ by $x = \chi(y, \xi^{(y)})$, where $\xi^{(y)} = (\xi_1^{(y)}, \dots, \xi_m^{(y)}) \in \varpi_y \subseteq \mathbb{R}^m$ is the nuisance variable. We denote the random variable for $\xi^{(y)}$ by Ξ_y; i.e., $\Xi_y(\omega_y) = \xi^{(y)}$ where $\omega_y \in \Omega_y$ is the element of the sample space Ω_y of the nuisance variable, conditioned on $Y = y$. Then, we denote the random variables for X and Z_l^s conditioned on $Y = y$ by X_y and $Z_{l,y}^s$: $X_y(\omega_y) = \chi(y, \Xi_y(\omega_y)) \in \mathcal{X}$ and $Z_{l,y}^s = \phi_l^s \circ X_y$. For any $l \in [D]$ and $y \in \mathcal{Y}$, we define the sensitivity $c_l^y(\phi_l^s)$ of the trained encoder ϕ_l^s with respect to the nuisance variable $\xi^{(y)}$ by the number such that for all $i \in [m]$, $c_l^y(\phi_l^s) \geq \sup_{\xi_1^{(y)}, \dots, \xi_{i-1}^{(y)}, \xi_i^{(y)}, \tilde{\xi}_i^{(y)}, \xi_{i+1}^{(y)}, \dots, \xi_m^{(y)}} |\log p_y((\phi_l^s \circ \chi_y)(\xi_1^{(y)}, \dots, \xi_{i-1}^{(y)}, \xi_i^{(y)}, \xi_{i+1}^{(y)}, \dots, \xi_m^{(y)})) - \log p_y((\phi_l^s \circ \chi_y)(\xi_1^{(y)}, \dots, \xi_{i-1}^{(y)}, \tilde{\xi}_i^{(y)}, \xi_{i+1}^{(y)}, \dots, \xi_m^{(y)}))|$, where $\chi_y(\xi^{(y)}) = \chi(y, \xi^{(y)})$ and $p_y(q) = \mathbb{P}(Z_{l,y}^s = q)$.

For any $l \in [D+1]$ and $\lambda_l > 0$, define

$$C_{\lambda_l, l} = \frac{1}{e^{\lambda_l H(\phi_l^{\mathbf{S}})}} \sum_{q \in \mathcal{M}_l} (\mathbb{P}(\phi_l^{\mathbf{S}} = q))^{1-\lambda_l}, \tag{14}$$

where $H(\phi_l^{\mathbf{S}})$ is the entropy of the random variable $\phi_l^{\mathbf{S}}$. We define the set of the latent variable per class by $\mathcal{Z}_{l,y}^s = \{(\phi_l^s \circ \chi_y)(\xi^{(y)}) : \xi^{(y)} \in \varpi_y\}$. For any $\gamma > 0$, we then define a (typical) subset $\mathcal{Z}_{\gamma,l,y}^s$ (of the set $\mathcal{Z}_{l,y}^s$) by $\mathcal{Z}_{\gamma,y}^{s,l} = \{z \in \mathcal{Z}_{l,y}^s : -\log \mathbb{P}(Z_{l,y}^s = z) - H(Z_{l,y}^s) \leq c_l^y(\phi_l^s) \sqrt{\frac{m \ln(\sqrt{n}/\gamma)}{2}}\}$. Let us write the element of $\mathcal{Z}_{\gamma,y}^{s,l}$ by $\mathcal{Z}_{\gamma,y}^{s,l} = \{a_1^{l,y}, \dots, a_{T_y^l}^{l,y}\}$ where $T_y^l = |\mathcal{Z}_{\gamma,y}^{s,l}|$. Finally, define maximum training loss $\mathcal{L}(f^s) = \max_{i \in \{1,\dots,n\}} \ell(f^s(x_i), y_i)$.

A.1.2 DETAILS OF OTHER TERMS

In Theorem 1, we have that $G_1^l(q) = \frac{\mathcal{L}(f^s)\sqrt{2\gamma_l |\mathcal{Y}|}}{n^{1/4}} \sqrt{q + \ln(2|\mathcal{Y}|/\delta)} + \gamma_l \mathcal{R}(f^s)$, $\mathcal{G}_2^l = G_2^l \ln(2) + \ln(2|\mathcal{Y}|/\delta)$, $G_3^l = \max_{y \in \mathcal{Y}} \sum_{k=1}^{T_y^l} \ell(g_l^s(a_k^{l,y}), y) \sqrt{2|\mathcal{Y}| \mathbb{P}(Z_{l,y}^s = a_k^{l,y})}$, and $G_2^l = \mathbb{E}_y[c_l^y(\phi_l^s)] \sqrt{\frac{m \ln(\frac{\sqrt{n}}{\gamma_l})}{2}} + H(Z_l^s | X, Y)$.

In Theorem 2, the definitions of $G_1^l(q), G_2^l, G_3^l$ are the same as in Theorem 1, and we have that $\zeta = (I(\phi_l^{\mathbf{S}}; \mathbf{S}) + G_4^l) \ln(2) + \ln(2|\mathcal{D}|)$, $\widehat{\mathcal{G}}_2^l = \left(G_2^l + G_4^l\right) \ln(2) + \ln(4|\mathcal{Y}||\mathcal{D}|/\delta)$, $\check{\mathcal{G}}_2^l = G_4^l \ln(2) + \ln(2/\delta)$, and $G_4^l = \frac{1}{\lambda_l} \ln \frac{C_{\lambda_l, l} |\mathcal{D}|}{\delta} + H(\phi_l^{\mathbf{S}} | \mathbf{S})$.

Proposition 2 below shows that G_3^l can be bounded by a constant value, which is much smaller than and independent of the size of the set $\mathcal{Z}_{\gamma,l,y}^s$.

Proposition 2. *Let $l \in \{1, \dots, D\}$. Let $v_k(y) = \ell(g_l^s(a_{j_k}^{l,y}), y)^2 \mathbb{P}(Z_{l,y}^s = a_{j_k}^{l,y})$ where $k \mapsto j_k$ is a permutation of the index such that $v_1(y) \geq v_2(y) \geq \cdots \geq v_{T_y^l}(y)$. If there exist some constants $\alpha_y \geq 1$ and $\beta_y, C_y > 0$ such that $v_k(y) \leq C_y e^{-(k/\beta_y)^{\alpha_y}}$, then*

$$G_3^l \leq \sqrt{2|\mathcal{Y}|} \max_{y \in \mathcal{Y}} \left(\sqrt{v_1(y)} \lceil \tilde{\beta}_y \rceil + (C_y \tilde{\beta}_y)/(\alpha_y e) \right), \tag{15}$$

without assuming that ϕ_l^s is fixed independently of the training dataset s, where $\tilde{\beta}_y = 2^{1/\alpha_y} \beta_y$.

Proof. The proof is provided in appendix B.8. □

Proposition 3 shows that the value of $\ln C_{\lambda_l,l}$ (recall from (14)) in the formula of G_4^l can be bounded by a constant value independently of $\ln |\mathcal{M}_l|$ and is much smaller than $\ln |\mathcal{M}_l|$ and $H(\phi_l^{\mathbf{S}})$:

Proposition 3. *Let $l \in \{1, \dots, D+1\}$. We denote $N = |\mathcal{M}_l|$, and enumerate $\mathcal{M}_l$ as $q_1, q_2, q_3, \cdots, q_N$ with decreasing probability, i.e. $p_i = \mathbb{P}(\phi_l^{\mathbf{S}} = q_i)$ and $p_1 \geq p_2 \geq \cdots \geq p_N$.*

1. *If p_i decays sufficiently fast, i.e., $p_i \leq C/i^\alpha$ with some $\alpha > 1$ and $C \geq 1$, then for $0 < \lambda_l < 1 - 1/\alpha$, both the entropy $H(\phi_l^{\mathbf{S}})$ and $C_{\lambda_l,l}$ are bounded and independent of N:*

$$H(\phi_l^{\mathbf{S}}) \leq 1 + C\alpha \left(\frac{\ln(2)}{2^\alpha} + \frac{\ln(3)}{3^\alpha} + \frac{3^{1-\alpha}((a-1)\ln(3)+1)}{(\alpha-1)^2} \right),$$

$$C_{\lambda_l,l} \leq C^{1-\lambda_l} \frac{\alpha(1-\lambda_l)}{\alpha(1-\lambda_l)-1}.$$

2. *If p_i decays slowly, i.e., $p_i = c_i/(Zi^\alpha)$ with $0 \leq \alpha < 1$ and $0 < c \leq c_i \leq C$ where Z is the normalization constant, then the entropy $H(\phi_l^{\mathbf{S}})$ grows as $\ln(N) + \mathcal{O}(1)$ where $\mathcal{O}(1)$ depends only on α, but $C_{\lambda_l,l}$ is bounded and independent of N as:*

$$C_{\lambda_l,l} \leq (\ln(1-(1-\lambda_l)\alpha) - (1-2\lambda_l)\ln(1-\alpha)) + (2-\lambda_l)\ln(C/c) + \frac{C}{c(1-\alpha)}.$$

Proof. The proof is provided in appendix B.9. □

We now discuss the factors $G_1^l(q)$ and G_2^l in Theorem 1. The formula of $G_1^l(q)$ is simplified as $G_1^l(q) = \gamma_l$ for any $q \in \mathbb{R}_{\geq 0}$ in a common scenario of deep learning where we use the 0-1 loss (to measure generalization) and have zero training error. This is because $\mathcal{L}(f^s) = 0$ and $\mathcal{R}(f^s) \leq 1$ for the scenario. In the formula of G_2, we have $H(Z_l^s|X,Y) = 0$ if the function ϕ_l^s is deterministic, which is the typical case for deep neural networks, because ϕ_l^s is the function used at inference or test time as opposed to training time (when dropout for example can be used). When the function ϕ_l^s is stochastic, we have $H(Z_l^s|X,Y) = \mathcal{O}(1)$ as $n \to \infty$. The networks can be stochastic, for example, with randomization defenses against adversarial attacks (Xie et al., 2018; Pinot et al., 2019; 2020; Levine & Feizi, 2020) or noise injections (Goldfeld et al., 2019). The value of $\mathbb{E}_y[c_l^y(\phi_l^s)]$ in the formula of G_2 measures the sensitivity with respect to the nuisance variable $\xi^{(y)}$; i.e., minimizing this value should result in better generalization, which is consistent with Theorem 1. The sensitivity $c_l^y(\phi_l^s)$ is a measure on the single final encoder ϕ_l^s; i.e., increasing the complexity of hypothesis spaces does not imply an increase in this value.

All the discussions and results, including Proposition 2, on the factors $G_1^l(q), G_2^l$, and G_3^l in Theorem 1 hold true for these factors in Theorem 2 (because we do not assume the use of the fixed encoder for these). Accordingly, we now discuss the new factor, G_4, in Theorem 2. The value of $\ln C_{\lambda_l,l}$ in the formula of G_4^l is analyzed in Proposition 3. In the formula of G_4, $H(\phi_l^{\mathbf{S}}|\mathbf{S})$ measures the randomness of algorithm $\mathcal{A}_l$. To understand this, let us consider a real-world experiment with a coin tossing. We can model the coin tossing by a stochastic model (by saying that coin tossing has 50-50 chance of getting heads and tails) or by a deterministic model to predict the exact outcome with an exact initial condition of the physical system. Similarly, we can model a single real-world algorithm with a stochastic model $\mathcal{A}_l$ (by saying that something has some random chances) or a deterministic model $\mathcal{A}_l$ with the exact initial condition, which is the random seed in the numerical experiments. That is, as in any mathematical theories and symbols, $\mathcal{A}_l$ is a theoretical placeholder with its mathematical definition; i.e., $\mathcal{A}_l$ does *not* have one-to-one correspondence to a real-world

algorithm implemented in experiments. In other words, given a single real-world algorithm, there are many different ways to model the real-world algorithm and different ways result in different $\mathcal{A}_l$. For example, let us fix the real-world algorithm implemented in experiments to be one with dropout (Srivastava et al., 2014) and stochastic gradient descent (SGD). At this point, $\mathcal{A}_l$ in Theorem 2 is not fully determined yet and we can choose $\mathcal{A}_l$ differently for the same real-world algorithm by modeling the real-world differently. For instance, we can model the one with dropout and SGD as a stochastic algorithm or as a deterministic algorithm given a fixed random seed in practice. Thus, we can set $\mathcal{A}_l$ in 2 to be either a stochastic algorithm or a deterministic algorithm for the exact same real-world and the same fixed algorithm implemented in experiments. If we set $\mathcal{A}_l$ to be a deterministic algorithm with a fixed seed, then we have $H(\phi_l^{\mathbf{S}}|\mathbf{S}) = 0$. If we set $\mathcal{A}_l$ to be a stochastic algorithm, then we increase $H(\phi_l^{\mathbf{S}}|\mathbf{S})$ but we can potentially decrease $I(\phi_l^{\mathbf{S}};\mathbf{S})$ since the extra randomness can potentially reduce the mutual information of $\phi_l^{\mathbf{S}}$ and $\mathbf{S}$. Thus, there is a trade-off in how we model the real-world via $\mathcal{A}_l$ and we cannot reduce the bound arbitrarily. Our theorems allow to instantiate our bounds with both deterministic and stochastic views of the learning algorithms, without changing the real-world algorithms.

More generally, a randomized algorithm can be defined as a deterministic algorithm with an additional input that consists of a sequence of random bits (Hromkovič, 2004). Here, the sequence of random bits corresponds to the sequence of random seeds in the numerical experiments with SGD. In other words, on the one hand, we can model SGD as a stochastic process when we analyze a set of experiments with SGD over a set of random seeds that are generated randomly. On the other hand, we can model SGD as a deterministic process when we analyze one experiment with SGD for one random seed. Moreover, as Hromkovič (2004) explains, we can bridge those two cases by modeling SGD as a deterministic algorithm with its additional inputs being the seed; then (1) it is deterministic for each seed, and (2) we can recover the stochastic model by considering a sequence of the randomly generated seeds. If we analyze one experiment of SGD for one random seed, then we have a deterministic algorithm, and a typical worst-case analysis provides a guarantee on the SGD with the worst seed. But, if we analyze a set of experiments of SGD over a set of random seeds that are generated randomly, then we have a stochastic algorithm, and we can analyze its expected performance or high-probability guarantee w.r.t. the random seeds.

To formally treat the learning algorithm $\mathcal{A}_l$ as a stochastic one, we replace $\mathbf{S}$ with $\tilde{\mathbf{S}}$ in eq. (8) where $\tilde{\mathbf{S}}(\omega, \omega') = (\mathbf{S}(\omega), \omega')$ with ω and ω' being elements of the sample spaces for $\mathbf{S}$ and $\mathcal{A}_l$ respectively. Similarly, when the encoder ϕ_l^s is stochastic, we replace X with $\tilde{X}$ in eq. (6) where $\tilde{X}(\omega, \omega') = (X(\omega), \omega')$ with ω and ω' being elements of the sample spaces for X and ϕ_l^s respectively. All of the proofs work in any of these cases.

A.2 On the application to The Case of Infinite Mutual Information

Section 3.3 discusses a way to apply a sample complexity bound with mutual information to the cases of infinite mutual information by using binning methods. This section considers a more general method of computing the mutual information to achieve the following goal: we demonstrate that a theoretical work on a bound with mutual information is an important and sensible research area more generally beyond our paper, even for the cases of infinite mutual information. This section also provides theoretical justifications on previous methods of computing mutual information even for the case of deterministic neural networks with continuous random variables with injective activations (Shwartz-Ziv & Tishby, 2017; Saxe et al., 2019; Chelombiev et al., 2019). We use the notation of $\phi^s = \phi_l^s$ and $g^s = g_l^s$ for a fixed l in this subsection.

This is based on the following simple observation: we can bound the generalization error of a given encoder, $\mathrm{G}[\tilde{\phi}^s]$, by using the generalization bound of another encoder, $\mathrm{B}_\delta[\phi^s]$, if we add the term measuring a distance between the two encoders, $\mathrm{D}(\phi^s, \tilde{\phi}^s)$. This is formalized in Remark 2:

Remark 2. Define $\mathrm{G}[\phi^s] = \mathbb{E}_{X,Y}[\ell_g(\phi^s(X), Y)] - \frac{1}{n}\sum_{i=1}^n \ell_g(\phi^s(x_i), y_i)$ and $\mathrm{L}[\phi^s] = \ell_g(\phi^s(X), Y)$ where $\ell_g(\phi^s(X), Y) = \ell((g^s \circ \phi^s)(X), Y)$. Suppose that for any $\delta > 0$, $\mathbb{P}(\mathrm{G}[\phi^s] \leq \mathrm{B}_\delta[\phi^s]) \geq 1 - \delta$ for some functional B_δ and that $\mathbb{P}_{X,Y}(|\mathrm{L}[\phi^s] - \mathrm{L}[\tilde{\phi}^s]| \leq \mathrm{D}(\phi^s, \tilde{\phi}^s)) = 1$ for some functional D. Then, for any $\delta > 0$, with at least probability $1 - \delta$,

$$\mathrm{G}[\tilde{\phi}^s] \leq \mathrm{B}_\delta[\phi^s] + 2\mathrm{D}(\phi^s, \tilde{\phi}^s). \tag{16}$$

Proof. Since $\mathbb{P}(|\mathrm{L}[\phi^s] - \mathrm{L}[\tilde{\phi}^s]| \leq \mathrm{D}(\phi^s, \tilde{\phi}^s)) = 1$, we have with probability one, $\mathrm{G}[\tilde{\phi}^s] \leq \mathrm{G}[\phi^s] + 2\mathrm{D}(\phi^s, \tilde{\phi}^s)$. Since $\mathbb{P}(\mathrm{G}[\phi^s] \leq \mathrm{B}[\phi^s]) \geq 1 - \delta$, we have with at least probability $1 - \delta$, $\mathrm{G}[\tilde{\phi}^s] \leq \mathrm{G}[\phi^s] + 2\mathrm{D}(\phi^s, \tilde{\phi}^s) \leq \mathrm{B}_\delta[\phi^s] + 2\mathrm{D}(\phi^s, \tilde{\phi}^s)$. □

Here, let us set $\mathrm{B}_\delta[\phi^s]$ to be a generalization bound on ϕ^s with mutual information. Then, given an original model $\tilde{\phi}^s$, its direct bound $\mathrm{B}_\delta[\tilde{\phi}^s]$ can be infinite since its mutual information can be infinite, for example, for deterministic neural networks $\tilde{\phi}^s$ with sigmoid activations for continuous random variables. However, instead of using its direct bound $\mathrm{B}_\delta[\tilde{\phi}^s]$, we can bound the generalization error of the original model $\tilde{\phi}^s$ by invoking Remark 2 to use the bound $\mathrm{B}_\delta[\phi^s]$ of another model $\phi^s \neq \tilde{\phi}^s$ such that ϕ^s has finite mutual information and $\mathrm{D}(\phi^s, \tilde{\phi}^s)$ is small.

Indeed, this is a theoretical formalization of what is implicitly done in practice when we compute mutual information of deterministic models. That is, in practice, we often compute the mutual information of the original model $\tilde{\phi}^s$ by computing the mutual information of another model ϕ^s where ϕ^s is a binning version of $\tilde{\phi}^s$ or a noise injected version of $\tilde{\phi}^s$ with kernel density estimation (Shwartz-Ziv & Tishby, 2017; Saxe et al., 2019; Chelombiev et al., 2019).

Indeed, all of such methods of computing mutual information in experiments are theoretically valid and meaningful based on our results in Section 3.3 and Remark 2 along with Proposition 4 below, even for the case of mutual information being infinite for the original model $\tilde{\phi}^s$.

As a concrete example, we now study the case when ϕ^s is obtained from $\tilde{\phi}^s$ by injecting noise, i.e. $\phi^s(x) = \tilde{\phi}^s(x) + \lambda\vartheta$, where $\vartheta \sim \mathcal{N}(0, \mathbb{I}_d/d)$ is the Gaussian noise (d is the dimension of the intermediate output $\tilde{\phi}^s(x)$):

Proposition 4. *Let $\phi^s(x) = \tilde{\phi}^s(x) + \lambda\vartheta$, where $\vartheta \sim \mathcal{N}(0, \mathbb{I}_d/d)$. Let L be the Lipschitz constant of the function $q \mapsto \ell_g(q, Y)$ y w.r.t. the metric induced by $\|\cdot\|_2$ almost surely. Then, we can take $D(\phi^s, \tilde{\phi}^s) = \lambda L\|\vartheta\|_2$, and with probability at least $1 - 2\delta$,*

$$\mathrm{G}[\tilde{\phi}^s] \leq \mathrm{B}_\delta[\phi^s] + 2\lambda L\sqrt{\log(2/\delta)}. \tag{17}$$

Proof. Since the function $q \mapsto \ell(g_l^s(q), Y)$ is Lipschitz almost surely, we have that with probability one,

$$|\ell_g(\phi^s(X), Y) - \ell_g(\tilde{\phi}^s(X), Y)| \leq |\ell_g(\tilde{\phi}^s(X) + \lambda\vartheta, Y) - \ell_g(\tilde{\phi}^s(X), Y)| \leq \lambda L\|\vartheta\|_2.$$

Thus, we can take $D(\phi^s, \tilde{\phi}^s) = \lambda L\|\vartheta\|_2$. Since $\vartheta \sim \mathcal{N}(0, \mathbb{I}_d/d)$ is a Gaussian vector, by Bernstein inequality, $\mathbb{P}(\|\vartheta\|_2 \geq t) \leq 2e^{-t^2/2}$. If we take $t = 2\sqrt{\log(2/\delta)}$, we get $D(\phi^s, \tilde{\phi}^s) \leq \lambda L\|\vartheta\|_2 \leq 2\lambda L\sqrt{\log(2/\delta)}$ with probability $1 - \delta$. Thus, Proposition 4 follows from Remark 2 by taking union bounds. □

In Proposition 4, let us set $\mathrm{B}_\delta[\phi^s]$ to be a generalization bound on ϕ^s with mutual information $I(Z; X)$ where $Z = \phi^s \circ X$. Then, by the construction of $\phi^s(x) = \tilde{\phi}^s(x) + \lambda\vartheta$, the output is stochastic, and the mutual information $I(Z; X)$ in $\mathrm{B}_\delta[\phi^s]$ is bounded, although $I(\tilde{Z}; X)$ with $\tilde{Z} = \tilde{\phi}^s \circ X$ can be infinite. Moreover, there is a trade-off between the two terms on the right-hand side of (17): injecting more noise by increasing λ reduces the mutual information $I(Z; X)$ in $\mathrm{B}_\delta[\phi^s]$, but increases error $2\lambda L\sqrt{\log(2/\delta)}$. Thus, we cannot arbitrarily change values of the bounds of the original model $\mathrm{G}[\tilde{\phi}^s]$ by choosing different methods of computing the mutual information even for the case of deterministic neural networks with continuous random variables with injective activations.

A.3 On comparisons with previous information-theoretic bounds

We discuss the difference between our bounds and the previous information-theoretic bounds (Xu & Raginsky, 2017; Bassily et al., 2018) in Section 3.2; e.g., the previous bounds do not utilize the information bottleneck term. In this subsection, we provide additional discussion on the relation between them.

We first note that Theorem 2 recovers the previous bounds if we set $\mathcal{D} = \{D+1\}$. If $\mathcal{D} = \{D+1\}$, then our bound in Theorem 2 removes $I(X; Z_l^s|Y)$ and only keeps $I(\phi_{D+1}^{\mathbf{S}}; \mathbf{S}) = I(f^{\mathbf{S}}; \mathbf{S})$, resulting in the previous bounds. This is because the hypothesis space of the decoder after the output layer is always a singleton (since there is no learnable parameter) and thus there is no need of "(information) bottleneck" to avoid overfitting of such decoder. Indeed, the previous bounds only consider the setting where the hypothesis space of the decoder is a singleton; e.g., g is the identity function. In the previous bounds, since the hypothesis space of the decoder g is singleton, there is no need for the encoder to provide a bottleneck to control the complexity of the hypothesis space of the decoder. In contrast, we consider non-singleton hypothesis spaces of decoders and utilize the information bottleneck of the encoder to control the complexity of the decoder. This also illustrates the difficulty to prove our sample complexity bounds with the information bottleneck where we need to consider the non-singleton hypothesis space for the decoder.

Another challenge of proving our bounds comes from the fact that we need to efficiently utilize different sources of randomness while the previous bounds only consider the single source of randomness; i.e., $f^{\mathbf{S}} = \mathcal{A}_{D+1} \circ \mathbf{S}$ is a random variable through the randomness of training data $\mathbf{S}$ (and potentially of algorithm $\mathcal{A}_{D+1}$) whereas $Z_l^s = \phi_l^s \circ X$ is a random variable through the randomness of the new unseen input X (and potentially of encoder ϕ_l^s). Thus, $I(X; Z_l^s|Y)$ and $I(f^{\mathbf{S}}; \mathbf{S})$ measures different types of mutual information with the different sources of randomness. Our bound needs to utilize both types of randomness efficiently while the previous bound only uses the randomness of $\mathbf{S}$.

The main factor $I(X; Z_l^s|Y) + I(\phi_l^{\mathbf{S}}; \mathbf{S})$ in Theorem 2 captures the novel tradeoff between the two types of mutual information. It tells us that as we minimize the information bottleneck $I(X; Z_l^s|Y)$ by optimizing ϕ_l^s based on the training data s, we must pay the price of mutual information $I(\phi_l^{\mathbf{S}}; \mathbf{S})$. If $\phi_l^{\mathbf{S}}$ depends more on $\mathbf{S}$, then we can more easily minimize the information bottleneck $I(X; Z_l^s|Y)$ (while minimizing the training loss for s), which comes at the cost of increasing $I(\phi_l^{\mathbf{S}}; \mathbf{S})$. This trade-off is not captured by any of previous bounds.

As a result of utilizing the both types of randomness, we show in Section 4 that the main factor $I(X; Z_l^s|Y) + I(\phi_l^{\mathbf{S}}; \mathbf{S})$ in our bound is a better predictor than the main factor $I(f^{\mathbf{S}}; \mathbf{S})$ in the previous bounds.

A.4 On the standard arguments for proving the conjecture

The previous work (Shwartz-Ziv et al., 2019) provided the arguments of using the Probably Approximately Correct (PAC) bound for a finite hypothesis space $\mathcal{H}$ to obtain $\tilde{\mathcal{O}}(\sqrt{(\log|\mathcal{H}|)/n})$ (Shalev-Shwartz & Ben-David, 2014) and bounding its cardinality $|\mathcal{H}|$ via $H(Z_l^s)$. However, this argument results in the exponential factor $2^{I(X;Z_l^s)}$ as in Conjecture 1.

B Proofs

B.1 Overview of Proofs of Theorems

Before providing complete proofs, we first provide a overview of the proofs of Theorem 1–2. Let $l \in [D]$. We first prove two properties of the typical set of Z_l, Lemma 1 and Lemma 2 (in appendix B.2), by combining a standard proof used in information theory and the McDiarmid's inequality. A typical set is a concept in information theory and we utilize the properties of a typical set to obtain the information-theoretic bounds. To achieve this, Lemma 3 (in appendix B.2) decomposes the generalization gap into four terms as $\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^n \ell(f^s(x_i), y_i) = \mathrm{A} + \mathrm{B} + \mathrm{C} + \mathrm{D}$, where the one term A corresponds to the case of X being in the typical set, while other three terms B, C, and D are for the case of X being outside of the typical set. The rest of the proof of Theorem 1 analyzes each of these terms (with Lemma 1 and Lemma 2), proving that A and $\mathrm{B} + \mathrm{C} + \mathrm{D}$ are bounded by the first term and the second term on the right-hand side of eq. (11), respectively. That is, we show $\mathrm{C} + \mathrm{D} \leq \frac{\gamma_l \mathcal{R}(f^s)}{\sqrt{n}}$ in Lemma 4 (in appendix B.2) by invoking Lemma 1. Lemma 5 (in appendix B.2) then bounds the terms A and B by recasting the problem into that of multinomial distributions and by incorporating Lemma 2 into the concentration inequality of multinomial distributions.

Lemmas 1–4 (in appendix B.2) are carefully proven for the trained encoder ϕ_l^s instead of a hypothesis space of encoders ϕ_l. This is achieved by combining deterministic decompositions and probabilistic bounds with respect to the randomness of new fresh samples X instead of the training data $\mathbf{S}$. In contrast, Lemma 5 (in appendix B.2) is proven for a hypothesis space Φ of encoders using the randomness of $\mathbf{S}$, where Φ must be independent of s. These decompositions and probabilistic bounds for different sample spaces enable the exponential improvement over the previous bounds. Combining Lemmas 3-5 (in appendix B.2) produces Lemma 6, which proves Theorem 1 by setting the hypothesis space as $\Phi = \{\phi_l^s\}$ where ϕ_l^s is fixed independently of s.

The standard proof techniques result in the exponential factor $2^{I(X;Z_l^s)}$ as in Conjecture 1 (see appendix A for more details). This paper provides a novel proof technique to avoid the exponential factor. Compared to arguments for Conjecture 1, our proof discards the non-mathematical arguments regarding the typical set, keeps track of all the effects of the approximation and non-typicality rigorously, and discards the assumption of the input dimension approaching infinity with an ergodic Markov random field.

Another main challenge in proving our main result, Theorem 2, is avoiding the dependence on the hypothesis space for the value of $I(X; Z_l^s|Y)$. That is, with a relatively simpler proof, we could prove a similar bound with $\sup_{\phi_l \in \Phi_l} I(X; \phi_l \circ X|Y)$ where Φ_l is a fixed hypothesis space of the encoder ϕ_l. However, this dependence on the hypothesis space is not preferred since enlarging the hypothesis space can increase the value, whereas the value of $I(X; Z_l^s)$ in our bound is independent of the hypothesis space given the final hypothesis ϕ_l^s.

We carefully construct and prove our key lemmas in the following subsection, which enables us to avoid the dependence over the entire hypothesis space and the exponential factor.

B.2 Proofs of Key Lemmas

We use the notation of $\ln = \log_e$ and $\log = \log_2$. Fix $l \in \{1, \dots, D\}$ throughout this section. For the simplicity of the notation, we write $Z = Z_l^s$ and $Z_y = Z_{l,y}^s$ in the following; we must to be always aware of the dependence on s for related variables. We recall that

$$Z_y = \phi_l^s \circ X_y.$$

We write $\xi^{(y)} \in \varpi_y \subseteq \mathbb{R}^m$, and define the set of the latent variable per class by

$$\mathcal{Z}_y = \left\{ (\phi_l^s \circ \chi_y)(\xi^{(y)}) : \xi^{(y)} \in \varpi_y \right\}.$$

For any $\gamma > 0$, we then define the typical subset $\mathcal{Z}_{\gamma,y}^s$ of the set $\mathcal{Z}_y$ by

$$\mathcal{Z}_{\gamma,y}^s = \left\{ z \in \mathcal{Z}_y : -\log \mathbb{P}(Z_y = z) - H(Z_y) \le c_l^y(\phi_l^s) \sqrt{\frac{m \ln(\sqrt{n}/\gamma)}{2}} \right\}.$$

Then, for any set A and any function φ, we have that

$$\begin{aligned} \mathbb{P}(Z \in A|Y = y) = \mathbb{P}(Z_y \in A) &= \mathbb{P}(\{\omega_y \in \Omega_y : Z_y(\omega_y) \in A\}) \\ &= \mathbb{P}(\{\omega_y \in \Omega_y : (\phi_l^s \circ \chi_y)(\Xi_y(\omega_y)) \in A\}) \\ &= \mathbb{P}((\phi_l^s \circ \chi_y \circ \Xi_y) \in A), \end{aligned}$$

and

$$\begin{aligned} \mathbb{P}((\varphi \circ Z) > 0|Y = y) = \mathbb{P}((\varphi \circ Z_y) > 0) &= \mathbb{P}(\{\omega_y \in \Omega_y : \varphi(Z_y(\omega_y)) > 0\}) \\ &= \mathbb{P}(\{\omega_y \in \Omega_y : \varphi((\phi_l^s \circ \chi_y)(\Xi_y(\omega_y))) > 0\}) \\ &= \mathbb{P}((\varphi \circ \phi_l^s \circ \chi_y \circ \Xi_y) > 0). \end{aligned}$$

Thus, for example, we can write

$$\begin{aligned} \mathbb{P}(Z \notin \mathcal{Z}_{\gamma,y}^s|Y = y) &= \mathbb{P}\left((\phi_l^s \circ \chi_y \circ \Xi_y) \notin \mathcal{Z}_{\gamma,y}^s\right) \\ &= \mathbb{P}\left(\{\omega_y \in \Omega_y : -\log \mathbb{P}(Z_y = \phi_l^s(X_y(\omega_y))) - H(Z_y) > \epsilon\}\right) \\ &= \mathbb{P}\left(\left\{\omega_y \in \Omega_y : -\log \mathbb{P}\left(\{\omega_y' \in \Omega_y : Z_y(\omega_y') = Z_y(\omega_y)\}\right) - H(Z_y) > \epsilon\right\}\right), \end{aligned}$$

where $\epsilon = c_l^y(\phi_l^s) \sqrt{\frac{m \ln(\sqrt{n}/\gamma)}{2}}$.

B.2.1 PROBABILITY OF GOING OUTSIDE OF THE TYPICAL SUBSET

The following lemma shows that the conditional probability of going outside of $\mathcal{Z}_{\gamma,y}$ is bounded by $\frac{\gamma}{\sqrt{n}}$:

Lemma 1. *For any $\gamma > 0$, it holds that*

$$\mathbb{P}(Z \notin \mathcal{Z}^s_{\gamma,y} \mid Y = y) \leq \frac{\gamma}{\sqrt{n}}.$$

Proof. Fix $y \in \mathcal{Y}$. We then write $\xi = \xi^{(y)}$ for the simplicity of the notation. We now consider the statistical property of the function $\xi \mapsto -\log \mathbb{P}(Z_y = \phi^s_l(\chi(y, \xi)))$. That is, in the following, we will apply McDiarmid's inequality w.r.t. the sample space $\omega_y \in \Omega_y$ to the following function:

$$\xi \mapsto -\log \mathbb{P}(Z_y = \phi^s_l(\chi(y,\xi))) = -\log \mathbb{P}(\{\omega'_y \in \Omega_y : Z_y(\omega'_y) = \phi^s_l(\chi(y,\xi))\}).$$

For the simpler notation, define the function p_y by

$$p_y(q) = \mathbb{P}(Z_y = q).$$

Then, we can rewrite the above function of ξ as

$$\xi = (\xi_1, \ldots, \xi_m) \mapsto -\log p_y(\phi^s_l(\chi(y,\xi))).$$

We also define

$$\tilde{\mathcal{Z}}^s_{\epsilon,y} = \{z \in \mathcal{Z}_y : -\log p_y(z) - H(Z) \leq \epsilon\}.$$

For any (h, φ) and $t = h(q)$ with a probability mass function p, since $p(t) = \sum_{q \in h^{-1}(t)} p(q)$,

$$\begin{aligned}
\mathbb{E}_{t\sim p}[\varphi(t)] = \sum_t \varphi(t)p(t) &= \sum_t \varphi(t) \sum_{q \in h^{-1}(t)} p(q) \\
&= \sum_t \sum_{q \in h^{-1}(t)} \varphi(t)p(q) \\
&= \sum_t \sum_{q \in h^{-1}(t)} \varphi(h(q))p(q) \\
&= \sum_q \varphi(h(q))p(q) = \mathbb{E}_{q\sim p}[\varphi(h(q))].
\end{aligned}$$

Thus, by choosing $q = \xi_y$, $h(q) = \phi^s_l(\chi(y,q))$, and $\varphi(t) = -\log p_y(t)$, we have that

$$\mathbb{E}_{\Xi_y}[-\log p_y(\phi^s_l(\chi(y,\Xi_y)))] = \mathbb{E}_q[\varphi(h(q))] = \mathbb{E}_t[\varphi(t)] = \mathbb{E}_{Z_y}[-\log p_y(Z_y)] = H(Z_y).$$

Thus, by using McDiarmid's inequality,

$$\mathbb{P}_{\Xi_y}(-\log p_y((\phi^s_l \circ \chi_y)(\Xi_y)) - H(Z_y) \geq \epsilon) \leq \exp\left(-\frac{2\epsilon^2}{m c^y_l(\phi^s_l)^2}\right).$$

By setting $\delta = \exp\left(-\frac{2\epsilon^2}{c^y_l(\phi^s_l)^2}\right)$ and solving for ϵ, we set

$$\epsilon = c^y_l(\phi^S_l)\sqrt{\frac{m\ln(1/\delta)}{2}},$$

with which

$$\begin{aligned}
\mathbb{P}(Z \notin \tilde{\mathcal{Z}}^s_{\epsilon,y} \mid Y = y) &= \mathbb{P}_{\Xi_y}\left((\phi^s_l \circ \chi_y)(\Xi_y) \notin \tilde{\mathcal{Z}}^s_{\epsilon,y}\right) \\
&= \mathbb{P}_{\Xi_y}(-\log p_y((\phi^s_l \circ \chi_y)(\Xi_y)) - H(Z_y) > \epsilon) \\
&\leq \mathbb{P}_{\Xi_y}(-\log p_y((\phi^s_l \circ \chi_y)(\Xi_y)) - H(Z_y) \geq \epsilon) \leq \delta.
\end{aligned}$$

Therefore, by setting $\delta = \frac{\gamma}{\sqrt{n}}$ and accordingly $\epsilon = c^y_l(\phi^s_l)\sqrt{\frac{m\ln(1/\delta)}{2}} = c^y_l(\phi^s_l)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}}$, we have proven the desired statement, since $\tilde{\mathcal{Z}}^s_{\epsilon,y} = \mathcal{Z}^s_{\gamma,y}$ when $\epsilon = c^y_l(\phi^s_l)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}}$. □

B.2.2 SIZE OF THE TYPICAL SUBSET

The following lemmas bounds the size of the subset $\mathcal{Z}^s_{\gamma,y}$:

Lemma 2. *For any $\gamma > 0$,*

$$|\mathcal{Z}^s_{\gamma,y}| \leq 2^{H_y(Z_y)+c^y_l(\phi^S_l)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}}}.$$

Proof. Set $\epsilon = c^y_l(\phi^s_l)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}}$. We define the function p_y by $p_y(q) = \mathbb{P}(Z_y = q)$. Then, from the definition of $\mathcal{Z}^s_{\gamma,y}$, we have that for any $a \in \mathcal{Z}^s_{\gamma,y}$,

$$\begin{aligned} -\log p_y(a) - H(Z_y) \leq \epsilon &\iff -\log p_y(a) \leq H(Z_y) + \epsilon \\ &\iff -\left(H(Z_y) + \epsilon\right) \leq \log p_y(a) \\ &\iff 2^{-H(Z_y)-\epsilon} \leq p_y(a). \end{aligned}$$

Using $2^{-H(Z_y)-\epsilon} \leq p_y(a) = \mathbb{P}(Z_y = a)$ for all $a \in \mathcal{Z}^s_{\gamma,y}$,

$$1 \geq \mathbb{P}(Z_y \in \mathcal{Z}^s_{\gamma,y}) = \sum_{a\in\mathcal{Z}^s_{\gamma,y}} \mathbb{P}(Z_y = a) \geq \sum_{a\in\mathcal{Z}^s_{\gamma,y}} 2^{-H(Z_y)-\epsilon} = |\mathcal{Z}^s_{\gamma,y}|2^{-H(Z_y)-\epsilon}.$$

This implies that using $\epsilon = c^y_l(\phi^s_l)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}}$,

$$|\mathcal{Z}^s_{\gamma,y}| \leq 2^{H(Z_y)+\epsilon} = 2^{H(Z_y)+c^y_l(\phi^S_l)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}}}.$$

□

B.2.3 DECOMPOSITION OF EXPECTED LOSS USING THE TYPICAL SUBSET

Let us write

$$z_i = \phi^s_l(x_i) \in \mathcal{Z}_l \subseteq \mathbb{R}^{m_l},$$

and

$$\ell_l(q, y) = \ell(g^s_l(q), y).$$

Then, by the law of the unconscious statistician,

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^n \ell(f^s(x_i), y_i) = \mathbb{E}_{Z,Y}[\ell_l(Z, Y)] - \frac{1}{n}\sum_{i=1}^n \ell_l(z_i, y_i).$$

For simplicity of the notation, define $A_y = \mathcal{Z}^s_{\gamma,y}$. We now consider a partition of the space $\mathcal{Z}_l$ as $\mathcal{Z}_l = \{z \in A_y\} \cup \{z \notin A_y\}$. Fix an order and write the element of A_y by $A_y = \{a^y_1, \ldots, a^y_{T_y}\}$ where $T_y = |A_y| \leq 2^{H_y(\phi_l \circ X_y)+c^y_l(\phi^S_l)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}}}$ from the Lemma 2. We define $\mathcal{I}_y = \{i \in [n] : y_i = y\}$, $\tilde{\mathcal{I}}^y = \{i \in [n] : z_i \notin A_y, y_i = y\}$, $\mathcal{I}^y_k = \{i \in [n] : z_i = a^y_k, y_i = y\}$, $\tilde{\mathcal{Y}} = \{y \in \mathcal{Y} : |\tilde{\mathcal{I}}^y| \neq 0\}$, $\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y} \ell_l(z_i, y)q \triangleq 0$ for any q if $|\tilde{\mathcal{I}}^y| = 0$, and $\frac{1}{|\mathcal{I}^y_k|}\sum_{i\in\mathcal{I}^y_k} \ell_l(z_i, y)q \triangleq 0$ for any q if $|\mathcal{I}^y_k| = 0$. Here, for example, Z, a^y_k, A_y, $|\mathcal{I}^y_k|$, and $|\tilde{\mathcal{I}}^y|$ depend on the training dataset s through the function ϕ^s_l due to their definitions.

Using these, we can decompose the expected loss as in the following lemma:

Lemma 3. *The following holds (deterministically):*

$$\begin{aligned} &\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^n \ell(f^s(x_i), y_i) \qquad (18) \\ &= \sum_{y\in\tilde{\mathcal{Y}}} \frac{1}{|\tilde{\mathcal{I}}^y|} \sum_{i\in\tilde{\mathcal{I}}^y} \ell_l(z_i, y) \left(\mathbb{P}(Y = y, Z \notin A_y) - \frac{|\tilde{\mathcal{I}}^y|}{n}\right) \\ &\quad + \sum_{y\in\mathcal{Y}} \sum_{k=1}^{T_y} \ell_l(a^y_k, y) \left(\mathbb{P}(Y = y, Z = a^y_k) - \frac{|\mathcal{I}^y_k|}{n}\right) \end{aligned}$$

$$+\sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y,Z\notin A_y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y,Y=y]$$
$$-\sum_{y\in\tilde{\mathcal{Y}}}\mathbb{P}(Y=y,Z\notin A_y)\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y).$$

Proof. we can decompose the expected loss by using conditionals as

$$\mathbb{E}_{Z,Y}[\ell_l(Z,Y)]=\sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Y=y].$$

Furthermore, we can decompose the conditional expectation as

$$\begin{aligned}\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Y=y]&=\mathbb{P}(Z\notin A_y|Y=y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y,Y=y]\\&\quad+\mathbb{P}(Z\in A_y|Y=y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\in A_y,Y=y]\\&=\mathbb{P}(Z\notin A_y|Y=y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y,Y=y]\\&\quad+\sum_{k=1}^{T_y}\mathbb{P}(Z=a_k^y|Y=y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z=a_k^y,Y=y]\\&=\mathbb{P}(Z\notin A_y|Y=y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y,Y=y]\\&\quad+\sum_{k=1}^{T_y}\mathbb{P}(Z=a_k^y|Y=y)\ell_l(a_k^y,y)\end{aligned}$$

Summarising above,

$$\begin{aligned}\mathbb{E}_{Z,Y}[\ell_l(Z,Y)]&=\sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y,Z\notin A_y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y,Y=y]\\&\quad+\sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\mathbb{P}(Y=y,Z=a_k^y)\ell_l(a_k^y,y).\end{aligned}$$

Similarly, we can decompose the training loss as

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^{n}\ell_l(z_i,y_i)&=\frac{1}{n}\sum_{y\in\mathcal{Y}}\sum_{i\in\mathcal{I}_y}\ell_l(z_i,y)\\&=\frac{1}{n}\sum_{y\in\mathcal{Y}}\left(\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)+\sum_{k=1}^{T_y}\sum_{i\in\mathcal{I}_k^y}\ell_l(z_i,y)\right)\\&=\sum_{y\in\tilde{\mathcal{Y}}}\frac{|\tilde{\mathcal{I}}^y|}{n}\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)+\sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\frac{|\mathcal{I}_k^y|}{n}\ell_l(a_k,y)\end{aligned}$$

Using these, we now decompose the expected loss as follows:

$$\begin{aligned}&\mathbb{E}_{Z,Y}[\ell_l(Z,Y)]-\frac{1}{n}\sum_{i=1}^{n}\ell_l(z_i,y_i)\\&=\sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y,Z\notin A_y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y,Y=y]\\&\quad+\sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\mathbb{P}(Y=y,Z=a_k^y)\ell_l(a_k^y,y)-\frac{1}{n}\sum_{i=1}^{n}\ell_l(z_i,y_i)\\&\quad\pm\sum_{y\in\tilde{\mathcal{Y}}}\mathbb{P}(Y=y,Z\notin A_y)\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)\pm\sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\frac{|\mathcal{I}_k^y|}{n}\ell_l(a_k,y)\end{aligned}$$

By rearranging,

$$
\begin{aligned}
&\mathbb{E}_{Z,Y}[\ell_l(Z,Y)] - \frac{1}{n}\sum_{i=1}^{n}\ell_l(z_i,y_i) \\
&= \sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y, Z\notin A_y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y, Y=y] \\
&\quad - \sum_{y\in\tilde{\mathcal{Y}}}\mathbb{P}(Y=y, Z\notin A_y)\left(\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)\right) \\
&\quad + \sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\ell_l(a_k^y,y)\left(\mathbb{P}(Y=y,Z=a_k^y) - \frac{|\mathcal{I}_k^y|}{n}\right) \\
&\quad + \sum_{y\in\tilde{\mathcal{Y}}}\mathbb{P}(Y=y,Z\notin A_y)\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y) + \sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\frac{|\mathcal{I}_k^y|}{n}\ell_l(a_k,y) - \frac{1}{n}\sum_{i=1}^{n}\ell_l(z_i,y_i) \\
&= \sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y, Z\notin A_y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y, Y=y] \\
&\quad - \sum_{y\in\tilde{\mathcal{Y}}}\mathbb{P}(Y=y, Z\notin A_y)\left(\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)\right) \\
&\quad + \sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\ell_l(a_k^y,y)\left(\mathbb{P}(Y=y,Z=a_k^y) - \frac{|\mathcal{I}_k^y|}{n}\right) \\
&\quad + \sum_{y\in\tilde{\mathcal{Y}}}\mathbb{P}(Y=y,Z\notin A_y)\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y) + \sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\frac{|\mathcal{I}_k^y|}{n}\ell_l(a_k,y) \\
&\quad - \sum_{y\in\tilde{\mathcal{Y}}}\frac{|\tilde{\mathcal{I}}^y|}{n}\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y) - \sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\frac{|\mathcal{I}_k^y|}{n}\ell_l(a_k,y)
\end{aligned}
$$

By combining the relevant terms,

$$
\begin{aligned}
&\mathbb{E}_{Z,Y}[\ell_l(Z,Y)] - \frac{1}{n}\sum_{i=1}^{n}\ell_l(z_i,y_i) \\
&= \sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y, Z\notin A_y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y, Y=y] \\
&\quad - \sum_{y\in\tilde{\mathcal{Y}}}\mathbb{P}(Y=y, Z\notin A_y)\left(\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)\right) \\
&\quad + \sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\ell_l(a_k^y,y)\left(\mathbb{P}(Y=y,Z=a_k^y) - \frac{|\mathcal{I}_k^y|}{n}\right) \\
&\quad + \sum_{y\in\tilde{\mathcal{Y}}}\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)\left(\mathbb{P}(Y=y,Z\notin A_y) - \frac{|\tilde{\mathcal{I}}^y|}{n}\right) + \sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\frac{|\mathcal{I}_k^y|}{n}\left(\ell_l(a_k,y) - \ell_l(a_k,y)\right) \\
&= \sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y, Z\notin A_y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y, Y=y] \\
&\quad - \sum_{y\in\tilde{\mathcal{Y}}}\mathbb{P}(Y=y, Z\notin A_y)\left(\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)\right)
\end{aligned}
$$

$$+\sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\ell_l(a_k^y,y)\left(\mathbb{P}(Y=y,Z=a_k^y)-\frac{|\mathcal{I}_k^y|}{n}\right)$$
$$+\sum_{y\in\tilde{\mathcal{Y}}}\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)\left(\mathbb{P}(Y=y,Z\notin A_y)-\frac{|\tilde{\mathcal{I}}^y|}{n}\right)$$

This implies the desired statement. □

B.2.4 Bounding the third and forth terms in the decomposition

Define

$$R_y=\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y,Y=y].$$

Then, the following lemma bounds the third and forth terms in the decomposition of (18) from the previous subsection:

Lemma 4. *For any $\gamma>0$, the following holds:*

$$\sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y)\frac{\gamma R_y}{\sqrt{n}}\geq\sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y,Z\notin A_y)\mathbb{E}_{Z,Y}[\ell_l(Z,Y)|Z\notin A_y,Y=y]$$
$$-\sum_{y\in\tilde{\mathcal{Y}}}\mathbb{P}(Y=y,Z\notin A_y)\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y). \tag{19}$$

Proof. Recalling the definition of $A_y=\mathcal{Z}_{\gamma,y}^s$, the third term can be written as

$$\sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y,Z\notin A_y)R_y=\sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y)\mathbb{P}(Z\notin\mathcal{Z}_{\gamma,y}^s|Y=y)R_y.$$

Then, using Lemma 1, for any $\gamma>0$,

$$\mathbb{P}(Z\notin\mathcal{Z}_{\gamma,y}^s|Y=y)\leq\frac{\gamma}{\sqrt{n}}.$$

Since $\sum_{y\in\tilde{\mathcal{Y}}}\mathbb{P}(Y=y,Z\notin A_y)\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)\geq 0$, combining these implies the desired statement. □

B.2.5 Bounding the first and second term in the decomposition

Let Φ be fixed such that Φ is independent of s, while Φ can depend on the underlying data distribution. The following lemma probabilistically bounds the first and second term in the decomposition of (18):

Lemma 5. *If $\phi_l^s\in\Phi$, for any $\gamma>0$ and $\delta>0$, with probability at least $1-\delta$, the following holds:*

$$\sum_{y\in\tilde{\mathcal{Y}}}\frac{1}{|\tilde{\mathcal{I}}^y|}\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)\left(\mathbb{P}(Y=y,Z\notin A_y)-\frac{|\tilde{\mathcal{I}}^y|}{n}\right) \tag{20}$$
$$\leq\left(\sum_{y\in\tilde{\mathcal{Y}}}\sqrt{\mathbb{P}(Z\notin\mathcal{Z}_{\gamma,y}^s,Y=y)\frac{\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)}{|\tilde{\mathcal{I}}^y|}}\right)\sqrt{\frac{2\ln(2|\Phi||\mathcal{Y}|/\delta)}{n}},\ \textit{and,}$$
$$\sum_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\ell_l(a_k^y,y)\left(\mathbb{P}(Y=y,Z=a_k^y)-\frac{|\mathcal{I}_k^y|}{n}\right)$$
$$\leq\sum_{y\in\mathcal{Y}}\left(\sum_{k=1}^{T_y}\ell_l(a_k^y,y)\sqrt{\mathbb{P}(Z=a_k^y,Y=y)}\right)\sqrt{\frac{2\left(I(X_y;Z_y)+G_2^y\right)\ln(2)+2\ln(2|\Phi||\mathcal{Y}|/\delta)}{n}}.$$

where

$$G_2^y=c_l^y(\phi_l^s)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}}+H(Z_y|X_y).$$

Proof. Let $\gamma > 0$ fixed. Define

$$\mathcal{X}_y = \left\{ \chi_y(\xi^{(y)}) : \xi^{(y)} \in \varpi_y \right\},$$

and

$$\hat{A}_y(\phi_l) = \left\{ x \in \mathcal{X}_y : -\log \mathbb{P}(Z_y = \phi_l(x)) - H(Z_y) \leq c_l^y(\phi_l) \sqrt{\frac{m \ln(\sqrt{n}/\gamma)}{2}} \right\}.$$

For each ϕ_l, write the element of $\hat{A}_y(\phi_l)$ by $\hat{A}_y(\phi_l) = \{\hat{a}_1^y(\phi_l), \ldots, \hat{a}^y_{\hat{T}_y(\phi_l)}(\phi_l)\}$ (with a fixed order) where $\hat{T}_y(\phi_l) = |\hat{A}_y(\phi_l)|$. Moreover, we define

$$\hat{\mathcal{I}}_k^y(\phi_l) = \begin{cases} \{i \in [n] : \phi_l(x_i) = \hat{a}_k^y(\phi_l), y_i = y\} & \text{if } k \in [\hat{T}_y(\phi_l)] \\ \{i \in [n] : \phi_l(x_i) \notin \hat{A}_y(\phi_l), y_i = y\} & \text{if } k = \hat{T}_y(\phi_l) + 1. \end{cases}$$

These are defined such that the previously defined notations are recovered when we set $\phi_l = \phi_l^s$ as

$$\begin{aligned} &\mathcal{Z}^s_{\gamma,y} = \hat{A}_y(\phi_l^s), \quad A_y = \hat{A}_y(\phi_l^s), \\ &(a_1^y, \ldots, a_T^y) = (\hat{a}_1^y(\phi_l^s), \ldots, \hat{a}^y_{\hat{T}_y(\phi_l^S)}(\phi_l^s)), \quad \mathcal{I}_k^y = \hat{\mathcal{I}}_k^y(\phi_l^s), \\ &\tilde{\mathcal{I}}^y = \hat{\mathcal{I}}^y_{\hat{T}_y(\phi_l^S)+1}(\phi_l^s), \quad T_y = \hat{T}_y(\phi_l^s). \end{aligned} \tag{21}$$

We begin with bounding terms for a fixed encoder, before extending it to the case of encoders learned from the training set. Let ϕ_l fixed and define

$$p_k^y = \begin{cases} \mathbb{P}((\phi_l \circ X) = \hat{a}_k^y(\phi_l), Y = y) & \text{if } k \in [\hat{T}_y(\phi_l)] \\ \mathbb{P}((\phi_l \circ X) \notin \hat{A}_y(\phi_l), Y = y) & \text{if } k = \hat{T}_y(\phi_l) + 1. \end{cases}$$

Let $y \in \mathcal{Y}$ and $k \in [\hat{T}_y(\phi_l) + 1]$. Then, we first prove the following statement: for any $\delta > 0$, with probability at least $1 - \delta$,

$$p_k^y - \frac{|\hat{\mathcal{I}}_k^y(\phi_l)|}{n} \leq \sqrt{\frac{2p_k^y \ln(1/\delta)}{n}}. \tag{22}$$

To prove this statement, fix $y \in \mathcal{Y}$ and $k \in [\hat{T}_y(\phi_l) + 1]$. Let us write $\hat{\mathcal{I}}_k = \hat{\mathcal{I}}_k^y(\phi_l)$ and $p_k = p_k^y$. If $p_k = 0$, then the desired statement holds trivially because $p_k - \frac{|\hat{\mathcal{I}}_k|}{n} = -\frac{|\hat{\mathcal{I}}_k|}{n} \leq \sqrt{\frac{2p_k \ln(1/\delta)}{n}}$ where $\frac{|\hat{\mathcal{I}}_k|}{n} = 0$ and $\sqrt{\frac{2p_i \ln(1/\delta)}{n}} = 0$. Thus, for the rest, we consider the case where $p_k \neq 0$. We notice that $(|\hat{\mathcal{I}}_1|, \ldots, |\hat{\mathcal{I}}_{T+1}|)$ follows the multinomial distribution with parameter n and $(p_1, \ldots, p_{T+1})$. Thus, we invoke Lemma 3 of (Kawaguchi et al., 2022) with $\bar{a}_i = 1$ and $\bar{a}_j = 0$ for all $j \neq i$ (which satisfies $\sum_{i=1}^K \bar{a}_i p_i \neq 0$ since $p_i \neq 0$), yielding that for any $M > 0$,

$$\mathbb{P}\left(p_k - \frac{|\hat{\mathcal{I}}_k|}{n} > M \right) \leq \exp\left(-\frac{nM^2}{2p_k} \right).$$

By setting $M = \sqrt{\frac{2p_i \ln(1/\delta)}{n}}$,

$$\mathbb{P}\left(p_k - \frac{|\hat{\mathcal{I}}_k|}{n} > \sqrt{\frac{2p_k \ln(1/\delta)}{n}} \right) \leq \delta.$$

This proves the statement of (22). Using (22), we can bound the first and second terms for a fixed ϕ_l as follows. For the first term with a fixed ϕ_l, using (22), by taking union bounds over all $y \in \mathcal{Y}$, we have that for any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $y \in \mathcal{Y}$:

$$\mathbb{P}(\phi_l(X) \notin \hat{A}_y(\phi_l), Y = y) - \frac{|\hat{\mathcal{I}}^y_{\hat{T}_y(\phi_l)+1}(\phi_l)|}{n} \tag{23}$$

$$\leq \sqrt{\frac{2\mathbb{P}(\phi_l(X) \notin \hat{A}_y(\phi_l), Y = y) \ln(|\mathcal{Y}|/\delta)}{n}}.$$

For the second term with a fixed ϕ_l, using (22), by taking union bounds over all $y \in \mathcal{Y}$ and all $k \in [\hat{T}_y(\phi_l)]$, we have that for any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $y \in \mathcal{Y}$ and all $k \in [\hat{T}_y(\phi_l)]$,

$$\mathbb{P}(\phi_l(X) = \hat{a}_k^y(\phi_l), Y = y) - \frac{|\hat{\mathcal{I}}_k^y(\phi_l)|}{n}$$
$$\leq \sqrt{\mathbb{P}(\phi_l(X) = \hat{a}_k^y(\phi_l), Y = y)} \sqrt{\frac{2 \ln(|\mathcal{Y}|\hat{T}_y(\phi_l)/\delta)}{n}}.$$

We now extend the results for the case of encoders learned from the training set; i.e., ϕ_l is no longer fixed. By taking union bounds with the previous two bounds, we have that for any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $\phi_l \in \Phi$:

$$\mathbb{P}(\phi_l(X) \notin \hat{A}_y(\phi_l), Y = y) - \frac{|\hat{\mathcal{I}}^y_{\hat{T}_y(\phi_l)+1}(\phi_l)|}{n}$$
$$\leq \sqrt{\frac{2\mathbb{P}(\phi_l(X) \notin \hat{A}_y(\phi_l), Y = y) \ln(2|\Phi||\mathcal{Y}|/\delta)}{n}},$$

and for all $k \in [\hat{T}_y(\phi_l)]$,

$$\mathbb{P}(\phi_l(X) = \hat{a}_k^y(\phi_l), Y = y) - \frac{|\hat{\mathcal{I}}_k^y(\phi_l)|}{n}$$
$$\leq \sqrt{\mathbb{P}(\phi_l(X) = \hat{a}_k^y(\phi_l), Y = y)} \sqrt{\frac{2 \ln(2|\Phi||\mathcal{Y}|\hat{T}_y(\phi_l)/\delta)}{n}}.$$

Thus, if $\phi_l^s \in \Phi$, then we have that for any $\delta > 0$, with probability at least $1-\delta$, the following holds:

$$\mathbb{P}(\phi_l^s(X) \notin \hat{A}_y(\phi_l^s), Y = y) - \frac{|\hat{\mathcal{I}}^y_{\hat{T}_y(\phi_l^S)+1}(\phi_l^s)|}{n}$$
$$\leq \sqrt{\frac{2\mathbb{P}(\phi_l^s(X) \notin \hat{A}_y(\phi_l^s), Y = y) \ln(2|\Phi||\mathcal{Y}|/\delta)}{n}}.$$

and for all $k \in [\hat{T}_y(\phi_l^s)]$,

$$\mathbb{P}(\phi_l^s(X) = \hat{a}_k^y(\phi_l^s), Y = y) - \frac{|\hat{\mathcal{I}}_k^y(\phi_l^s)|}{n}$$
$$\leq \sqrt{\mathbb{P}(\phi_l^s(X) = \hat{a}_k^y(\phi_l^s), Y = y)} \sqrt{\frac{2 \ln(2|\Phi||\mathcal{Y}|\hat{T}_y(\phi_l^s)/\delta)}{n}}.$$

By using (21), this means that if $\phi_l^s \in \Phi$, for any $\delta > 0$, with probability at least $1 - \delta$, the following holds:

$$\mathbb{P}(Z \notin \mathcal{Z}^s_{\gamma,y}, Y = y) - \frac{|\tilde{\mathcal{I}}^y|}{n} \leq \sqrt{\frac{2\mathbb{P}(Z \notin \mathcal{Z}^s_{\gamma,y}, Y = y) \ln(2|\Phi||\mathcal{Y}|/\delta)}{n}},$$

and for all $k \in [T_y]$,

$$\mathbb{P}(Z = a_k^y, Y = y) - \frac{|\mathcal{I}_k^y|}{n} \leq \sqrt{\mathbb{P}(Z = a_k^y, Y = y)} \sqrt{\frac{2 \ln(2|\Phi||\mathcal{Y}|T_y/\delta)}{n}}.$$

Since $\ell_l(z_i, y) \geq 0$ and $\ell_l(a_k^y, y) \geq 0$, this implies that if $\phi_l^s \in \Phi$, for any $\delta > 0$, with probability at least $1 - \delta$, the following holds:

$$\sum_{y \in \tilde{\mathcal{Y}}} \frac{1}{|\tilde{\mathcal{I}}^y|} \sum_{i \in \tilde{\mathcal{I}}^y} \ell_l(z_i, y) \left(\mathbb{P}(Y = y, Z \notin A_y) - \frac{|\tilde{\mathcal{I}}^y|}{n} \right)$$

$$\leq \left(\sum_{y \in \tilde{\mathcal{Y}}} \sqrt{\mathbb{P}(Z \notin \mathcal{Z}^s_{\gamma,y}, Y = y)} \frac{\sum_{i \in \tilde{\mathcal{I}}^y} \ell_l(z_i, y)}{|\tilde{\mathcal{I}}^y|} \right) \sqrt{\frac{2\ln(2|\Phi||\mathcal{Y}|/\delta)}{n}},$$

and for all $k \in [T_y]$,

$$\sum_{y \in \mathcal{Y}} \sum_{k=1}^{T_y} \ell_l(a^y_k, y) \left(\mathbb{P}(Y = y, Z = a^y_k) - \frac{|\mathcal{I}^y_k|}{n} \right)$$
$$\leq \sum_{y \in \mathcal{Y}} \left(\sum_{k=1}^{T_y} \ell_l(a^y_k, y) \sqrt{\mathbb{P}(Z = a^y_k, Y = y)} \right) \sqrt{\frac{2\ln(2|\Phi||\mathcal{Y}|T_y/\delta)}{n}}.$$

Here, using Lemma 2, we have that $T_y = |\mathcal{Z}^s_{\gamma,y}| \leq 2^{H(Z_y) + c^y_l(\phi^s_l)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}}}$. Thus,

$$\sqrt{\frac{2\ln(2|\Phi||\mathcal{Y}|T_y/\delta)}{n}} = \sqrt{\frac{2\ln(T_y) + 2\ln(2|\Phi||\mathcal{Y}|/\delta)}{n}}$$
$$\leq \sqrt{\frac{2\left(H(Z_y) + c^y_l(\phi^s_l)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}}\right)\ln(2) + 2\ln(2|\Phi||\mathcal{Y}|/\delta)}{n}}$$

Finally, since $H(Z_y) = I(X_y; Z_y) + H(Z_y|X_y)$, we have that

$$H(Z_y) + c^y_l(\phi^s_l)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}} = I(X_y; Z_y) + G^y_2.$$

Combining these, we have proven the desired statement of this lemma. □

B.2.6 COMBINE LEMMAS

By combining Lemmas 3, 4, and 5, we have proven the following statement:

Lemma 6. *Let* $l \in \{1, \ldots, D\}$. *If* $\phi^s_l \in \Phi$, *then for any* $\gamma > 0$ *and* $\delta > 0$, *with probability at least* $1 - \delta$, *the following holds:*

$$\mathbb{E}_{X,Y}[\ell((g^s_l \circ \phi^s_l)(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell((g^s_l \circ \phi^s_l)(x_i), y_i)$$
$$\leq G_3 \sqrt{\frac{I(X; Z|Y)\ln(2) + G_2\ln(2) + \ln(2|\Phi||\mathcal{Y}|/\delta)}{n}} + \frac{G_1(\ln|\Phi|)}{\sqrt{n}},$$

where

$$G_1(q) = \frac{\mathcal{L}(f^s)\sqrt{2\gamma|\mathcal{Y}|}}{n^{1/4}} \sqrt{\ln(q) + \ln(2|\mathcal{Y}|/\delta)} + \gamma\mathcal{R}(f^s),$$
$$G_2 = \mathbb{E}_y[c^y_l(\phi^s_l)] \sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}} + H(Z|X, Y),$$
$$G_3 = \max_{y \in \mathcal{Y}} \sum_{k=1}^{T_y} \ell_l(a^y_k, y) \sqrt{2|\mathcal{Y}|\mathbb{P}(Z = a^y_k|Y = y)}.$$

Proof. Define the radius of the expected loss R by

$$R = \mathbb{E}_y[R_y] = \mathbb{E}_y\left[\mathbb{E}_{Z,Y}[\ell_l(Z, Y)|Z \notin A_y, Y = y]\right], \tag{24}$$

and the maximum over y of the average training loss per y by

$$\hat{L}(f^s) = \max_{y \in \tilde{\mathcal{Y}}} \frac{1}{|\tilde{\mathcal{I}}^y|} \sum_{i \in \tilde{\mathcal{I}}^y} \ell_l(z_i, y) = \max_{y \in \tilde{\mathcal{Y}}} \frac{1}{|\tilde{\mathcal{I}}^y|} \sum_{i \in \tilde{\mathcal{I}}^y} \ell(f^s(x_i), y). \tag{25}$$

Let $l \in \{1, \ldots, D\}$. By combining Lemmas 3, 4, and 5, if $\phi_l^s \in \Phi$, then for any $\gamma > 0$ and $\delta > 0$, with probability at least $1 - \delta$, the following holds:

$$\begin{aligned}
&\mathbb{E}_{X,Y}[\ell((g_l^s \circ \phi_l^s)(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell((g_l^s \circ \phi_l^s)(x_i), y_i) \\
&\leq \sqrt{2}\sum_{y\in\mathcal{Y}} \left(\sum_{k=1}^{T_y} \ell_l(a_k^y, y)\sqrt{\mathbb{P}(Z = a_k^y, Y = y)}\right) \sqrt{\frac{(I(X_y; Z_y) + G_2^y)\ln(2) + \ln(2|\Phi||\mathcal{Y}|/\delta)}{n}} \\
&\quad + \left(\sum_{y\in\tilde{\mathcal{Y}}} \sqrt{\mathbb{P}(Z \notin \mathcal{Z}_{\gamma,y}^s, Y = y)} \frac{\sum_{i\in\tilde{\mathcal{I}}^y} \ell_l(z_i, y)}{|\tilde{\mathcal{I}}^y|}\right) \sqrt{\frac{2\ln(2|\Phi||\mathcal{Y}|/\delta)}{n}} + \sum_{y\in\mathcal{Y}} \mathbb{P}(Y = y)\frac{\gamma R_y}{\sqrt{n}}.
\end{aligned}$$

Define

$$\tilde{G}_3 = \max_{y\in\mathcal{Y}} \sqrt{2}\sum_{k=1}^{T_y} \ell_l(a_k^y, y)\sqrt{\mathbb{P}(Z = a_k^y | Y = y)}.$$

Then, we have

$$\begin{aligned}
&\sqrt{2}\left(\sum_{k=1}^{T_y} \ell_l(a_k^y, y)\sqrt{\mathbb{P}(Z = a_k^y, Y = y)}\right) \\
&= \sqrt{\mathbb{P}(Y = y)}\sqrt{2}\left(\sum_{k=1}^{T_y} \ell_l(a_k^y, y)\sqrt{\mathbb{P}(Z = a_k^y | Y = y)}\right) \\
&\leq \tilde{G}_3\sqrt{\mathbb{P}(Y = y)}
\end{aligned}$$

Using this and Jensen's inequality, we have that

$$\begin{aligned}
&\sqrt{2}\sum_{y\in\mathcal{Y}} \left(\sum_{k=1}^{T_y} \ell_l(a_k^y, y)\sqrt{\mathbb{P}(Z = a_k^y, Y = y)}\right) \sqrt{\frac{(I(X_y; Z_y) + G_2^y)\ln(2) + \ln(2|\Phi||\mathcal{Y}|/\delta)}{n}} \\
&\leq \tilde{G}_3 \sum_{y\in\mathcal{Y}} \frac{|\mathcal{Y}|}{|\mathcal{Y}|}\sqrt{\mathbb{P}(Y = y)}\sqrt{\frac{(I(X_y; Z_y) + G_2^y)\ln(2) + \ln(2|\Phi||\mathcal{Y}|/\delta)}{n}} \\
&\leq \tilde{G}_3|\mathcal{Y}|\sqrt{\sum_{y\in\mathcal{Y}} \frac{1}{|\mathcal{Y}|}\frac{\mathbb{P}(Y = y)\,(I(X_y; Z_y) + G_2^y)\ln(2) + \mathbb{P}(Y = y)\ln(2|\Phi||\mathcal{Y}|/\delta)}{n}} \\
&= \tilde{G}_3\sqrt{|\mathcal{Y}|}\sqrt{\frac{\sum_{y\in\mathcal{Y}} \mathbb{P}(Y = y)\,(I(X_y; Z_y) + G_2^y)\ln(2) + \sum_{y\in\mathcal{Y}} \mathbb{P}(Y = y)\ln(2|\Phi||\mathcal{Y}|/\delta)}{n}} \\
&= \tilde{G}_3\sqrt{|\mathcal{Y}|}\sqrt{\frac{(I(X; Z|Y) + G_2)\ln(2) + \ln(2|\Phi||\mathcal{Y}|/\delta)}{n}}
\end{aligned}$$

where

$$G_2 = \sum_{y\in\mathcal{Y}} \mathbb{P}(Y = y)G_2^y = \sum_{y\in\mathcal{Y}} \mathbb{P}(Y = y)\left(c_l^y(\phi_l^s)\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}} + H(Z_y|X_y)\right).$$

Moreover,

$$\sum_{y\in\mathcal{Y}} \mathbb{P}(Y = y)\frac{\gamma R_y}{\sqrt{n}} = \frac{\gamma}{\sqrt{n}}\sum_{y\in\mathcal{Y}} \mathbb{P}(Y = y)R_y = \frac{\gamma R}{\sqrt{n}}.$$

Using Lemma 1 and Jensen's inequality, since $\mathbb{P}_Z(Z \notin \mathcal{Z}_{\gamma,y}^S | Y = y) \leq \frac{\gamma}{\sqrt{n}}$,

$$\sum_{y\in\tilde{\mathcal{Y}}} \sqrt{\mathbb{P}(Z \notin \mathcal{Z}_{\gamma,y}^s, Y = y)} \frac{\sum_{i\in\tilde{\mathcal{I}}^y} \ell_l(z_i, y)}{|\tilde{\mathcal{I}}^y|}$$

$$
\begin{aligned}
&= \sum_{y\in\tilde{\mathcal{Y}}} \sqrt{\mathbb{P}(Z \notin \mathcal{Z}^s_{\gamma,y}|Y=y)}\sqrt{\mathbb{P}(Y=y)}\frac{\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)}{|\tilde{\mathcal{I}}^y|} \\
&\le \hat{L}(f^s)\frac{\sqrt{\gamma}}{n^{1/4}}\sum_{y\in\mathcal{Y}}\frac{|\mathcal{Y}|}{|\mathcal{Y}|}\sqrt{\mathbb{P}(Y=y)} \\
&\le \hat{L}(f^s)\frac{\sqrt{\gamma}}{n^{1/4}}|\mathcal{Y}|\sqrt{\sum_{y\in\mathcal{Y}}\frac{1}{|\mathcal{Y}|}\mathbb{P}(Y=y)} \\
&= \hat{L}(f^s)\frac{\sqrt{\gamma|\mathcal{Y}|}}{n^{1/4}}
\end{aligned}
$$

Thus, since $R \le \mathcal{R}(f^s)$ and $\hat{L}(f^s) \le \mathcal{L}(f^s)$,

$$
\begin{aligned}
\frac{G_1(\ln|\Phi|)}{\sqrt{n}} \ge &\left(\sum_{y\in\tilde{\mathcal{Y}}}\sqrt{\mathbb{P}(Z\notin\mathcal{Z}^s_{\gamma,y},Y=y)}\frac{\sum_{i\in\tilde{\mathcal{I}}^y}\ell_l(z_i,y)}{|\tilde{\mathcal{I}}^y|}\right)\sqrt{\frac{2\ln(2|\Phi||\mathcal{Y}|/\delta)}{n}} \\
&+\sum_{y\in\mathcal{Y}}\mathbb{P}(Y=y)\frac{\gamma R_y}{\sqrt{n}},
\end{aligned}
$$

where

$$
G_1(q) = \frac{\mathcal{L}(f^s)\sqrt{2\gamma|\mathcal{Y}|}}{n^{1/4}}\sqrt{q+\ln(2|\mathcal{Y}|/\delta)} + \gamma\mathcal{R}(f^s).
$$

Combining these imply the desired statement. □

B.3 Completing the Proof of Theorem 1 with Key Lemmas

Recall that we have proven the following lemma in the previous subsection:

Lemma 6. *Let $l \in \{1,\dots,D\}$. If $\phi^s_l \in \Phi$, then for any $\gamma > 0$ and $\delta > 0$, with probability at least $1-\delta$, the following holds:*

$$
\begin{aligned}
&\mathbb{E}_{X,Y}[\ell((g^s_l\circ\phi^s_l)(X),Y)] - \frac{1}{n}\sum_{i=1}^n \ell((g^s_l\circ\phi^s_l)(x_i),y_i) \\
&\le G_3\sqrt{\frac{I(X;Z|Y)\ln(2)+G_2\ln(2)+\ln(2|\Phi||\mathcal{Y}|/\delta)}{n}} + \frac{G_1(\ln|\Phi|)}{\sqrt{n}},
\end{aligned}
$$

where

$$
\begin{aligned}
G_1(q) &= \frac{\mathcal{L}(f^s)\sqrt{2\gamma|\mathcal{Y}|}}{n^{1/4}}\sqrt{\ln(q)+\ln(2|\mathcal{Y}|/\delta)} + \gamma\mathcal{R}(f^s), \\
G_2 &= \mathbb{E}_y[c^y_l(\phi^s_l)]\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}} + H(Z|X,Y), \\
G_3 &= \max_{y\in\mathcal{Y}}\sum_{k=1}^{T_y}\ell_l(a^y_k,y)\sqrt{2|\mathcal{Y}|\mathbb{P}(Z=a^y_k|Y=y)}.
\end{aligned}
$$

Theorem 2 directly follows from Lemma 6; i.e., we complete the proof of Theorem 2 using Lemma 6. Since ϕ^s_l is fixed independently of the training dataset s in Theorem 1, we can invoke Lemma 6 with $\Phi = \{\phi^s_l\}$, with which $|\Phi| = 1$ and $\phi^s_l \in \Phi$. Thus, by noticing that $f^s = g^s_l \circ \phi^s_l$ for any $l \in \{1,\dots,D\}$, Lemma 6 implies the desired statement. □

B.4 Completing the Proof of Theorem 2 with Key Lemmas

We complete the proof of Theorem 2 by extending Lemma 6 in the following.

B.4.1 FINDING A LIKELY SPACE OF ENCODER

Fix $l \in \{1, \ldots, D\}$ throughout this section. Let $\lambda = \lambda_l$ and $C_\lambda = C_{\lambda,l}$. Recall that $\mathcal{A}_l(s) \in \mathcal{M}_l$ and $|\mathcal{M}_l| < \infty$. For simplicity of notation, we define the random variable A_S by $A_S = \phi_l^{\mathbf{S}}$. For any $q \in \mathcal{M}_l$, we denote

$$p(q) = \mathbb{P}(A_S = q). \tag{26}$$

The entropy of the random variable A_S is given by

$$\mathbb{E}_{A_S}\left[-\log p(A_S)\right] = H(A_S).$$

Define the typical subset

$$\Phi_\epsilon^l = \left\{\phi_l \in \mathcal{M}_l : -\log \mathbb{P}(A_S = \phi_l) - H(A_S) \leq \epsilon\right\}.$$

The following proposition shows that the probability of going outside of the typical subset Φ_ϵ^l is bounded by δ when we take $\epsilon = (1/\lambda)\log(C_\lambda/\delta)$:

Lemma 7. *For any $\lambda > 0$, if we take $\epsilon = (1/\lambda)\ln(C_\lambda/\delta)$, then we have*

$$\mathbb{P}(\phi_l^{\mathbf{S}} \notin \Phi_\epsilon^l) \leq \delta, \tag{27}$$

and

$$|\Phi_\epsilon^l| \leq 2^{H(\phi_l^{\mathbf{S}})+\epsilon} = 2^{H(\phi_l^{\mathbf{S}})+\frac{1}{\lambda}\log\frac{C_\lambda}{\delta}}. \tag{28}$$

Proof. By the definition of the set Φ_ϵ^l, we have

$$\begin{aligned}
\mathbb{P}(A_S \notin \Phi_\epsilon^l) &= \mathbb{P}(q \in \mathcal{M}_l : -\log p(q) \geq H(A_S) + \epsilon) && (29)\\
&= \mathbb{P}(q \in \mathcal{M}_l : -\lambda \log p(q) \geq \lambda H(A_S) + \lambda\epsilon) && (30)\\
&= \mathbb{P}(q \in \mathcal{M}_l : p^{-\lambda}(q) \geq e^{\lambda H(A_S)+\lambda\epsilon}) && (31)\\
&\leq e^{-\lambda H(A_S)-\lambda\epsilon} \sum_{q\in\mathcal{M}_l} p^{-\lambda}(q)p(q) && (32)\\
&= \frac{C_\lambda}{e^{\lambda\epsilon}} = \delta. && (33)
\end{aligned}$$

Now we compute the size of Φ_ϵ^l. From the definition of Φ_ϵ^l, we have

$$\begin{aligned}
-\log p(\phi_l) - H(A_S) \leq \epsilon &\iff -\log p(\phi_l) \leq H(A_S) + \epsilon\\
&\iff -H(A_S) - \epsilon \leq \log p(\phi_l)\\
&\iff 2^{-H(A_S)-\epsilon} \leq p(\phi_l).
\end{aligned}$$

Using $2^{-H(A_S)-\epsilon} \leq p(\phi_l)$,

$$1 \geq \mathbb{P}_S(A_S \in \Phi_\epsilon^l) = \sum_{\phi_l\in\Phi_\epsilon^l} \mathbb{P}(A_S = \phi_l) \geq \sum_{\phi_l\in\Phi_\epsilon^l} 2^{-H(A_S)-\epsilon} = |\Phi_\epsilon^l| 2^{-H(A_S)-\epsilon}.$$

This implies that using $\epsilon = (1/\lambda)\ln(C_\lambda/\delta)$,

$$|\Phi_\epsilon^l| \leq 2^{H(A_S)+\frac{1}{\lambda}\ln\frac{C_\lambda}{\delta}}.$$

□

B.4.2 RESULT WITH FIXED LAYER INDEX

Combining Lemmas 6 and 7 implies the following lemma, which is a main result for a fixed layer index l:

Lemma 8. *Let $l \in \{1, \dots, D\}$. Then, for any $\gamma > 0$ and any $\delta > 0$, with probability at least $1 - \delta$, the following holds:*

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(f^s(x_i), y_i) \tag{34}$$
$$\leq G_3 \sqrt{\frac{\big(I(X;Z|Y) + I(\phi_l^{\mathbf{S}};\mathbf{S}) + G_2 + G_4\big)\ln(2) + \ln(4|\mathcal{Y}|/\delta)}{n}} + \frac{G_1(\tilde{q})}{\sqrt{n}}.$$

where $\tilde{q} = (I(\phi_l^{\mathbf{S}};\mathbf{S}) + G_4)\ln(2) + \ln(2)$,

$$G_1(\tilde{q}) = \frac{\mathcal{L}(f^s)\sqrt{2\gamma|\mathcal{Y}|}}{n^{1/4}}\sqrt{\tilde{q} + \ln(2|\mathcal{Y}|/\delta)} + \gamma\mathcal{R}(f^s),$$
$$G_2 = \mathbb{E}_y[c_l^y(\phi_l^s)]\sqrt{\frac{m\ln(\sqrt{n}/\gamma)}{2}} + H(Z|X,Y),$$
$$G_3 = \max_{y\in\mathcal{Y}} \sum_{k=1}^{T_y} \ell_l(a_k^y, y)\sqrt{2|\mathcal{Y}|\mathbb{P}(Z = a_k^y|Y = y)},$$
$$G_4 = \frac{1}{\lambda}\ln\frac{C_\lambda}{\delta} + H(\phi_l^{\mathbf{S}}|\mathbf{S}).$$

Proof. Fix $l \in \{1, \dots, D\}$. Let $\lambda > 0$ and $\epsilon = (1/\lambda)\ln(C_\lambda/\delta)$. Using Lemma 6, if $\phi_l^s \in \Phi_\epsilon^l$, then for any $\gamma > 0$ and $\delta > 0$, with probability at least $1 - \delta$, the following holds:

$$\mathbb{E}_{X,Y}[\ell((g_l^s \circ \phi_l^s)(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell((g_l^s \circ \phi_l^s)(x_i), y_i) \tag{35}$$
$$\leq G_3 \sqrt{\frac{(I(X;Z|Y) + G_2)\ln(2) + \ln(2|\Phi_\epsilon^l||\mathcal{Y}|/\delta)}{n}} + \frac{G_1(\ln|\Phi_\epsilon^l|)}{\sqrt{n}}.$$

From Lemma 7,

$$\mathbb{P}(A_S \notin \Phi_\epsilon^l) \leq \delta$$
$$\mathbb{P}_S(\phi_l^s \notin \Phi_\epsilon^l) \leq \bar{\delta}.$$

Thus, since $\mathbb{P}(A \cap B) \leq \mathbb{P}(B)$ and $\mathbb{P}(A \cap B) = \mathbb{P}(A)\mathbb{P}(A \mid B)$, we have that

$$\begin{aligned}
&\mathbb{P}_{\mathbf{S}}(\text{Inequality (35) holds}) \\
&\geq \mathbb{P}_{\mathbf{S}}(\phi_l^{\mathbf{S}} \in \Phi_\epsilon^l \bigcap \text{Inequality (35) holds}) \\
&= \mathbb{P}_{\mathbf{S}}(\phi_l^{\mathbf{S}} \in \Phi_\epsilon^l)\mathbb{P}_{\mathbf{S}}(\text{Inequality (35) holds} \mid \phi_l^{\mathbf{S}} \in \Phi_\epsilon^l) \\
&\geq \mathbb{P}_{\mathbf{S}}(\phi_l^{\mathbf{S}} \in \Phi_\epsilon^l)(1-\delta) \\
&\geq (1-\delta)(1-\delta) = 1 - 2\delta + \delta^2 \geq 1 - 2\delta.
\end{aligned}$$

Therefore, by setting $\delta = \frac{\delta'}{2}$, we have that for any $\delta' > 0$,

$$\mathbb{P}_{\mathbf{S}}(\text{Eq (35) holds}) \geq 1 - \delta'.$$

In other words, for any $\gamma > 0$ and $\delta > 0$, with probability at least $1 - \delta$, the following holds:

$$\mathbb{E}_{X,Y}[\ell((g_l^s \circ \phi_l^s)(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell((g_l^s \circ \phi_l^s)(x_i), y_i) \tag{36}$$
$$\leq G_3 \sqrt{\frac{(I(X;Z|Y) + G_2)\ln(2) + \ln(4|\Phi_\epsilon^l||\mathcal{Y}|/\delta)}{n}} + \frac{G_1(\ln 2|\Phi_\epsilon^l|)}{\sqrt{n}}.$$

From Lemma 7, we have $|\Phi_\epsilon^l| \leq 2^{H(\phi_l^{\mathbf{S}}) + \frac{1}{\lambda}\ln\frac{C_\lambda}{\delta}}$ and thus

$$\ln(4|\Phi_\epsilon^l||\mathcal{Y}|/\delta) = \ln(|\Phi_\epsilon^l|) + \ln(4|\mathcal{Y}|/\delta) \leq \left(H(\phi_l^{\mathbf{S}}) + \frac{1}{\lambda}\ln\frac{C_\lambda}{\delta}\right)\ln(2) + \ln(4|\mathcal{Y}|/\delta).$$

From the definition of the entropy, conditional entropy, and mutual information, we have that

$$H(\phi_l^{\mathbf{S}}) = I(\phi_l^{\mathbf{S}}; \mathbf{S}) + H(\phi_l^{\mathbf{S}}|\mathbf{S}).$$

Using this,

$$H(\phi_l^{\mathbf{S}}) + \frac{1}{\lambda} \ln \frac{C_\lambda}{\delta} = I(\phi_l^{\mathbf{S}}; \mathbf{S}) + G_4.$$

By combining these and noticing that $f^s = g_l^s \circ \phi_l^s$ for any $l \in \{1, \dots, D\}$, we have that for any $\gamma > 0$ and $\delta > 0$, with probability at least $1 - \delta$, the following holds:

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n} \sum_{i=1}^{n} \ell(f^s(x_i), y_i) \tag{37}$$
$$\leq G_3 \sqrt{\frac{\big(I(X;Z|Y) + I(\phi_l^{\mathbf{S}}; \mathbf{S}) + G_2 + G_4\big) \ln(2) + \ln(4|\mathcal{Y}|/\delta)}{n}} + \frac{G_1(\tilde{q})}{\sqrt{n}}.$$

□

B.4.3 Completing the Proof

We complete the proof of Theorem 2 using Lemma 8. Let $\gamma_l > 0$ and $\lambda_l > 0$ for all $l \in \{1, 2, \dots, D+1\}$. Recall that $f^s = g_l^s \circ \phi_l^s$ for any $l \in \{1, \dots, D\}$. Thus, by making the dependence of the layer index l explicit, Lemma 8 states that for any $\delta > 0$ and (fixed) $l \in \{1, \dots, D\}$, with probability at least $1 - \delta$,

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n} \sum_{i=1}^{n} \ell(f^s(x_i), y_i) \tag{38}$$
$$\leq G_3^l \sqrt{\frac{\big(I(X;Z_l^s|Y) + I(\phi_l^{\mathbf{S}}; \mathbf{S}) + G_2^l + G_4^l\big) \ln(2) + \ln(4|\mathcal{Y}|/\delta)}{n}} + \frac{G_1^l(\tilde{q})}{\sqrt{n}},$$

where $\tilde{q} = (I(\phi_l^{\mathbf{S}}; \mathbf{S}) + G_4) \ln(2) + \ln(2)$,

$$G_1^l(q) = \frac{\mathcal{L}(f^s)\sqrt{2\gamma_l|\mathcal{Y}|}}{n^{1/4}} \sqrt{q + \ln(2|\mathcal{Y}|/\delta)} + \gamma_l \mathcal{R}(f^s),$$
$$G_2^l = \mathbb{E}_y[c_l^y(\phi_l^s)] \sqrt{\frac{m \ln(\sqrt{n}/\gamma_l)}{2}} + H(Z_l^s|X,Y).$$
$$G_3^l = \max_{y \in \mathcal{Y}} \sum_{k=1}^{T_y} \ell_l(a_k^y, y) \sqrt{2|\mathcal{Y}| \mathbb{P}(Z = a_k^y | Y = y)},$$
$$\tilde{G}_4^l = \frac{1}{\lambda_l} \ln \frac{C_{\lambda_l, l}}{\delta} + H(\phi_l^{\mathbf{S}}|\mathbf{S}).$$

We now consider the case of $l = D+1$. Let $l = D+1$ and $\lambda_{D+1} > 0$. Fix $f = \phi_{D+1} \in \Phi_\epsilon^{D+1}$ with $\epsilon = (1/\lambda) \ln(C_{\lambda_{D+1}, D+1}/\delta)$. Then, by using Hoeffding's inequality, for any $\delta > 0$, with probability at least $1 - \delta$,

$$\mathbb{E}_{X,Y}[\ell(f(X), Y)] - \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) \leq \mathcal{R}(f) \sqrt{\frac{\ln(1/\delta)}{2n}}.$$

By taking union bounds over elements of Φ_ϵ^{D+1}, this implies that for any $\delta > 0$, with probability at least $1 - \delta$, the following holds for all $f \in \Phi_\epsilon^{D+1}$,

$$\mathbb{E}_{X,Y}[\ell(f(X), Y)] - \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) \leq \mathcal{R}(f) \sqrt{\frac{\ln(|\Phi_\epsilon^{D+1}|/\delta)}{2n}}.$$

This implies that for any $\delta > 0$, if $\phi_{D+1}^s \in \Phi_\epsilon^{D+1}$, then with probability at least $1 - \delta$,

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n} \sum_{i=1}^{n} \ell(f^s(x_i), y_i) \leq \mathcal{R}(f^s) \sqrt{\frac{\ln(|\Phi_\epsilon^{D+1}|/\delta)}{2n}}. \tag{39}$$

Here, from Lemma 7, we have that

$$\mathbb{P}(\phi_{D+1}^{\mathbf{S}} \notin \Phi_\epsilon^{D+1}) \leq \delta.$$

Since $\mathbb{P}(A \cap B) \leq \mathbb{P}(B)$ and $\mathbb{P}(A \cap B) = \mathbb{P}(A)\mathbb{P}(A \mid B)$, we have that

$$\begin{aligned}
&\mathbb{P}_{\mathbf{S}}(\text{Inequality (39) holds}) \\
&\geq \mathbb{P}_{\mathbf{S}}(\phi_{D+1}^{\mathbf{S}} \in \Phi_\epsilon^{D+1} \bigcap \text{Inequality (39) holds}) \\
&= \mathbb{P}_{\mathbf{S}}(\phi_{D+1}^{\mathbf{S}} \in \Phi_\epsilon^{D+1}) \mathbb{P}_{\mathbf{S}}(\text{Inequality (39) holds} \mid \phi_{D+1}^{\mathbf{S}} \in \Phi_\epsilon^{D+1}) \\
&\geq \mathbb{P}_{\mathbf{S}}(\phi_{D+1}^{\mathbf{S}} \in \Phi_\epsilon^{D+1})(1-\delta) \\
&\geq (1-\delta)(1-\delta) \\
&\geq 1 - 2\delta.
\end{aligned}$$

Therefore, by setting $\delta = \frac{\delta'}{2}$, we have that for any $\delta' > 0$,

$$\mathbb{P}_{\mathbf{S}}(\text{Eq (39) holds}) \geq 1 - \delta'.$$

In other words, for any $\delta' > 0$, with probability at least $1 - \delta'$,

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^n \ell(f^s(x_i), y_i) \leq \mathcal{R}(f^s)\sqrt{\frac{\ln(2|\Phi_\epsilon^{D+1}|/\delta')}{2n}}. \tag{40}$$

Here, from Lemma 7, we have that

$$|\Phi_\epsilon^{D+1}| \leq 2^{H(\phi_{D+1}^{\mathbf{S}}) + \frac{1}{\lambda_{D+1}} \log \frac{C_{\lambda_{D+1}, D+1}}{\delta}}.$$

Substituting this,

$$\begin{aligned}
\ln(2|\Phi_\epsilon^{D+1}|/\delta') &= \ln(|\Phi_\epsilon^{D+1}|) + \ln(2/\delta') \\
&\leq \left(H(\phi_{D+1}^{\mathbf{S}}) + \frac{1}{\lambda_{D+1}} \log \frac{C_{\lambda_{D+1}, D+1}}{\delta}\right) \ln(2) + \ln(2/\delta')
\end{aligned}$$

Using $H(\phi_{D+1}^{\mathbf{S}}) = I(\phi_{D+1}^{\mathbf{S}}; \mathbf{S}) + H(\phi_{D+1}^{\mathbf{S}} | \mathbf{S})$,

$$H(\phi_{D+1}^{\mathbf{S}}) + \frac{1}{\lambda_{D+1}} \log \frac{C_{\lambda_{D+1}, D+1}}{\delta} = I(\phi_{D+1}^{\mathbf{S}}; \mathbf{S}) + \tilde{G}_4^{D+1}.$$

Substituting these into (40), we have that for any $\delta > 0$, with probability at least $1 - \delta$,

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^n \ell(f^s(x_i), y_i) \leq \mathcal{R}(f^s)\sqrt{\frac{\left(I(\phi_{D+1}^{\mathbf{S}}; \mathbf{S}) + \tilde{G}_4^{D+1}\right)\ln(2) + \ln(2/\delta)}{2n}}. \tag{41}$$

By combining (38) and (41) with union bounds over $\mathcal{D}$, we have that for any $\delta > 0$ and $\mathcal{D} \subseteq \{1, 2, \ldots, D+1\}$, with probability at least $1 - \delta$, the following holds for all $l \in \mathcal{D}$:

$$\begin{aligned}
&\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^n \ell(f^s(x_i), y_i) \qquad (42) \\
&\leq \mathbb{1}\{l \neq D_+\}\left(G_3^l \sqrt{\frac{\left(I(X; Z_l^s | Y) + I(\phi_l^{\mathbf{S}}; \mathbf{S}) + G_2^l + G_4^l\right)\ln(2) + \ln(4|\mathcal{Y}||\mathcal{D}|/\delta)}{n}} + \frac{G_1^l}{\sqrt{n}}\right) \\
&\quad + \mathbb{1}\{l = D_+\}\mathcal{R}(f^s)\sqrt{\frac{\left(I(\phi_{D+1}^{\mathbf{S}}; \mathbf{S}) + G_4^{D+1}\right)\ln(2) + \ln(2/\delta)}{2n}},
\end{aligned}$$

where $D_+ = D + 1$,

$$G_4^l = \frac{1}{\lambda_l} \ln \frac{C_{\lambda_l, l}|\mathcal{D}|}{\delta} + H(\phi_l^{\mathbf{S}} | \mathbf{S}).$$

Since the right-hand side of this inequality holds for all $l \in \mathcal{D}$ and the left-hand side does not depend on l, this implies that for any $\delta > 0$ and $\mathcal{D} \subseteq \{1, 2, \ldots, D+1\}$, with probability at least $1-\delta$,

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(f^s(x_i), y_i) \leq \min_{l \in \mathcal{D}} Q_l, \tag{43}$$

$$\text{where } Q_l = \begin{cases} G_3^l \sqrt{\frac{\left(I(X;Z_l^s|Y) + I(\phi_l^{\mathbf{S}};\mathbf{S})\right)\ln(2) + \widehat{\mathcal{G}}_2^l}{n}} + \frac{G_1^l(\zeta)}{\sqrt{n}} & \text{if } l \leq D \\ \mathcal{R}(f^s)\sqrt{\frac{I(\phi_l^{\mathbf{S}};\mathbf{S})\ln(2) + \check{\mathcal{G}}_2^l}{2n}} & \text{if } l = D+1, \end{cases}$$

where $\zeta = (I(\phi_l^{\mathbf{S}};\mathbf{S}) + G_4^l)\ln(2) + \ln(2|\mathcal{D}|)$, $\widehat{\mathcal{G}}_2^l = \left(G_2^l + G_4^l\right)\ln(2) + \ln(4|\mathcal{Y}||\mathcal{D}|/\delta)$, $\check{\mathcal{G}}_2^l = G_4^l \ln(2) + \ln(2/\delta)$, and $G_4^l = \frac{1}{\lambda_l}\ln\frac{C_{\lambda_l,l}|\mathcal{D}|}{\delta} + H(\phi_l^{\mathbf{S}}|\mathbf{S})$.

□

B.5 Proof of Remark 1

The desired statement follows from

$$I(\theta_l^{\mathbf{S}};\mathbf{S}) + H(\theta_l^{\mathbf{S}}|\mathbf{S}) = H(\theta_l^{\mathbf{S}}) \geq H(\phi_{l,\theta_l^{\mathbf{S}}}) = H(\phi_l^{\mathbf{S}}) = I(\phi_l^{\mathbf{S}};\mathbf{S}) + H(\phi_l^{\mathbf{S}}|\mathbf{S}),$$

where the inequality holds because all the randomness of $\phi_{l,\theta_l^{\mathbf{S}}}$ comes from the randomness of $\theta_l^{\mathbf{S}} = \mathcal{A}_l^{\theta} \circ \mathbf{S}$ (where $\mathcal{A}_l^{\theta}$ is the version of $\mathcal{A}_l$ that outputs the parameter vector instead of the encoder function), and because one $\phi_{l,\theta_l^{\mathbf{S}}}$ corresponds to one or more $\theta_l^{\mathbf{S}}$; i.e., we have $\phi_{l,\theta_l^s} = \phi_{l,\bar{\theta}_l^s}$ whenever $\theta_l^s = \bar{\theta}_l^s$ and it is possible that $\phi_{l,\theta_l^s} = \phi_{l,\bar{\theta}_l^s}$ for $\theta_l^s \neq \bar{\theta}_l^s$. In other words, the desired statement does not hold only if $\phi_{l,\theta_l^s} \neq \phi_{l,\bar{\theta}_l^s}$ for some $\theta_l^s = \bar{\theta}_l^s$, which is not the case.

□

B.6 Proof of Corollary 1

Proof. Set $\phi_l^s = \mathcal{E}_l[\tilde{\phi}_l^s] \circ \tilde{\phi}_l^s$. Then, Theorems 1–2 hold true for this choice of encoder ϕ_l^s since this does not violate any assumption of Theorems 1–2. Thus, Theorems 1–2 hold with eq. (11) and eq. (12) in their original forms: i.e.,

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(f^s(x_i), y_i) \leq \hat{Q}_l, \text{ and,} \tag{44}$$

$$\mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(f^s(x_i), y_i) \leq \min_{l \in \mathcal{D}} Q_l,$$

Since $\mathbb{P}(|\ell((g_l^s \circ \tilde{\phi}_l^s)(X), Y) - \ell((g_l^s \circ \mathcal{E}_l[\tilde{\phi}_l^s] \circ \tilde{\phi}_l^s)(X), Y)| \leq C_l) = \mathbb{P}(|\ell(\tilde{f}^s(X), Y) - \ell(f^s(X), Y)| \leq C_l) = 1$, we have that with probability one,

$$\ell(\tilde{f}^s(x_i), y_i) = \ell(f^s(x_i), y_i) + (\ell(\tilde{f}^s(x), y) - \ell(f^s(x_i), y_i)) \leq \ell(f^s(x_i), y_i) + C_l. \tag{45}$$

Thus, with probability one,

$$\mathbb{E}_{X,Y}[\ell(\tilde{f}^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(\tilde{f}^s(x_i), y_i) \leq \mathbb{E}_{X,Y}[\ell(f^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(f^s(x_i), y_i) + 2C_l. \tag{46}$$

Combining eq. (44) and eq. (46) with union bounds concludes that Theorems 1–2 hold when we replace eq. (11) and eq. (12) by

$$\mathbb{E}_{X,Y}[\ell(\tilde{f}^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(\tilde{f}^s(x_i), y_i) \leq \hat{Q}_l + 2C_l, \text{ and,} \tag{47}$$

$$\mathbb{E}_{X,Y}[\ell(\tilde{f}^s(X), Y)] - \frac{1}{n}\sum_{i=1}^{n} \ell(\tilde{f}^s(x_i), y_i) \leq \min_{l \in \mathcal{D}} Q_l + 2C_l,$$

Finally, the values of $\hat{Q}_l$ and Q_l are finite since $|\mathcal{Z}_l^s| < \infty$ and $|\mathcal{M}_l| < \infty$; e.g., $|\mathcal{Z}_l^s| < \infty$ implies that $I(X; Z_l^s|Y) < \infty$. Thus, if $C_{\mathcal{E}} < \infty$, we have $\hat{Q}_l + 2C_l < \infty$ and $\min_{l \in \mathcal{D}} Q_l + 2C_l < \infty$. □

B.7 PROOF OF PROPOSITION 1

Proof. Let l be fixed and $\phi^s = \phi^s_l$. For deterministic neural networks, the intermediate output Z is a deterministic function of the input X, i.e. $Z = \phi^s(X)$. In this case the conditional mutual information between X and Z simplifies to the conditional entropy of Z:

$$I(X, Z|Y) = H(Z|Y) = H(\phi^s(X)|Y). \tag{48}$$

It has been proven in (Amjad & Geiger, 2019) that if X has absolutely continuous component, which has continous density on a compact set, and the activation is bi-Lipschitz or continuous differentiable with strictly positive derivative, then the entropy of $\phi^s(X)$ is infinite.

In the following, we first give some simple examples with ReLU activation where the entropy of $\phi^s(X)$ is finite for an initial intuition, and then we generalize the examples for more practical settings. Finally, we discuss generality and practicality of our construction.

Consider an arbitrary (continuous or discrete) distribution such that the distribution of $X|Y$ consists of several components (which may correspond to further subclasses). For simplicity, we assume that there are two components $\mathcal{C}_1$ and $\mathcal{C}_2$. We start with the linearly separable case where $\mathcal{C}_1$ and $\mathcal{C}_2$ are separated by a hyperplane $ax + b = 0$ with margin at least r. In other words $ax + b \geq r$ for $x \in \mathcal{C}_1$, and $ax + b \leq -r$ for $x \in \mathcal{C}_2$. Then the following simple one layer network

$$\sigma(ax + b + c) - \sigma(ax + b - c), \quad 0 < c \leq r \tag{49}$$

maps $x \in \mathcal{C}_1$ to $2c$ and $\mathcal{C}_2$ to 0. Thus, the output $Z = \phi^s(X)$ follows a Bernoulli distribution, which has bounded entropy. Thus, we have $I(X, Z|Y) < \infty$.

More generally, if $\mathcal{C}_1$ and $\mathcal{C}_2$ are separable, with margin at least r using some metric $d(\mathcal{C}_1, \mathcal{C}_2) \geq r$, we can take a Lipschitz function g w.r.t. this metric d with lipschitz constant $1/r$ such that it equals 0 on C_1 and equals 1 on C_2. By the universal approximation theory, ReLU neural network can approximate arbitrary continuous function to arbitrary precision as we increase the network size. In particular, there exists a finite-size ReLU neural network N such that $|N(x) - g(x)| \leq 1/8$. As a consequence, we have $N(x) \leq 1/8$ for $x \in \mathcal{C}_1$ and $N(x) \geq 7/8$ for $x \in \mathcal{C}_2$. We consider the following neural network:

$$\sigma(N - 1/2 + c) - \sigma(N - 1/2 - c), \quad 0 < c < 3/8, \tag{50}$$

which maps $x \in \mathcal{C}_1$ to $2c$ and $\mathcal{C}_2$ to 0. Thus, the output $Z = \phi^s(X)$ follows a Bernoulli distribution, which has bounded entropy. Thus, we have $I(X, Z|Y) < \infty$. Since the distribution in this general example is arbitrary except for the separable components, there exists infinitely many such distributions.

Finally, we observe that these examples are general and practical. First, the above proof works for any finite number of separable components instead of two components. Second, it is also observed in practice that trained neural networks behave like these examples discussed above, which maps different class to different points; this is sometimes referred as a neural collapse phenomenon (Papyan et al., 2020). □

B.8 PROOF OF PROPOSITION 2

We will use the following lemma to prove Proposition 2:

Lemma 9. *Let $v_1, \ldots, v_T \in \mathbb{R}$ such that $0 \leq v_k \leq Ce^{-(k/\beta)^\alpha}$ for some constants $\alpha \geq 1$ and $\beta, C > 0$. Then,*

$$\sum_{k=1}^{T} \sqrt{v_k} \leq \sum_{k=1}^{\lceil \tilde{\beta} \rceil} \sqrt{v_k} + \frac{C\tilde{\beta}}{\alpha e}$$

where $\tilde{\beta} = 2^{1/\alpha}\beta$.

Proof. Using the condition on v_k,

$$\sqrt{v_k} \leq \sqrt{Ce^{-(k/\beta)^\alpha}} = \sqrt{C}\sqrt{e^{-(k/\beta)^\alpha}} = \sqrt{C}e^{-\frac{k^\alpha}{2\beta^\alpha}} = \sqrt{C}e^{-(k/\tilde{\beta})^\alpha}$$

Then,

$$\sum_{k=1}^{T}\sqrt{v_k} = \sum_{k=1}^{\lceil\tilde{\beta}\rceil}\sqrt{v_k} + \sum_{k=\lceil\tilde{\beta}\rceil+1}^{T}\sqrt{v_k} \leq \sum_{k=1}^{\lceil\tilde{\beta}\rceil}\sqrt{v_k} + \sqrt{C}\sum_{k=\lceil\tilde{\beta}\rceil+1}^{T} e^{-(k/\tilde{\beta})^{\alpha}}$$

We now bound the last term by using integral as

$$\sum_{k=\lceil\tilde{\beta}\rceil+1}^{T} e^{-(k/\tilde{\beta})^{\alpha}} \leq \int_{\tilde{\beta}}^{\infty} e^{-(q/\tilde{\beta})^{\alpha}}dq = \frac{\tilde{\beta}}{\alpha}\int_{(\tilde{\beta}/\tilde{\beta})^{\alpha}}^{\infty} t^{\frac{1}{\alpha}-1}e^{-t}dt = \frac{\tilde{\beta}}{\alpha}\int_{1}^{\infty} t^{\frac{1}{\alpha}-1}e^{-t}dt$$

Here, since $\alpha \geq 1$ and $t \geq 1$ in the integral, we have $t^{\frac{1}{\alpha}-1} \leq 1$ in the integral. Thus,

$$\int_{1}^{\infty} t^{\frac{1}{\alpha}-1}e^{-t}dt \leq \int_{1}^{\infty} e^{-t}dt = e^{-1}.$$

By combining these, we have

$$\sum_{k=1}^{T}\sqrt{v_k} \leq \sum_{k=1}^{\lceil\tilde{\beta}\rceil}\sqrt{v_k} + \frac{C\tilde{\beta}}{\alpha e}$$

□

Using Lemma 9, we complete the proof of Proposition 2 in the following:

Proof of Proposition 2. Let $y \in \mathcal{Y}$ and $l \in \{1, \ldots, D\}$. To invoke Lemma 9, we rearrange the expression of G_3^l as

$$\begin{aligned} G_3^l &= \max_{y\in\mathcal{Y}} \sum_{k=1}^{T_y^l} \ell(g_l^s(a_k^{l,y}), y)\sqrt{2|\mathcal{Y}|\mathbb{P}(Z_{l,y}^s = a_k^{l,y})} \\ &\leq \sqrt{2|\mathcal{Y}|}\max_{y\in\mathcal{Y}} \sum_{k=1}^{T_y^l} \sqrt{\ell(g_l^s(a_k^{l,y}), y)^2\mathbb{P}(Z_{l,y}^s = a_k^{l,y})} \end{aligned}$$

Then, we invoke Lemma 9 with $v_k = v_k^{(y)} = \ell(g_l^s(a_k^{l,y}), y)^2\mathbb{P}(Z_{l,y}^s = a_k^{l,y})$, where we define $v_k^{(y)} = v_k(y)$. This implies that

$$\sum_{k=1}^{T_y^l} \sqrt{\ell(g_l^s(a_k^{l,y}), y)^2\mathbb{P}(Z_{l,y}^s = a_k^{l,y})} \leq \sum_{k=1}^{\lceil\tilde{\beta}_y\rceil} \sqrt{v_k^{(y)}} + \frac{C_y\tilde{\beta}_y}{\alpha_y e},$$

where $\tilde{\beta}_y = 2^{1/\alpha_y}\beta_y$. Thus,

$$G_3^l \leq \sqrt{2|\mathcal{Y}|}\max_{y\in\mathcal{Y}}\left(\sum_{k=1}^{\lceil\tilde{\beta}_y\rceil} \sqrt{v_k^{(y)}} + \frac{C_y\tilde{\beta}_y}{\alpha_y e}\right)$$

□

B.9 Proof of Proposition 3

Proof. Let $l \in \{1, 2, \ldots, D+1\}$ and let us write $\lambda = \lambda_l$ and $C_\lambda = C_{\lambda_l, l}$. We first note that the value of C_λ is always bounded as

$$C_\lambda \leq \sum_{q\in\mathcal{M}_l} (\mathbb{P}(\phi_l^{\mathbf{S}} = q))^{1-\lambda} \leq |\mathcal{M}_l|\left(\frac{1}{|\mathcal{M}_l|}\sum_{q\in\mathcal{M}_l}\mathbb{P}(\phi_l^{\mathbf{S}} = q)\right)^{1-\lambda} = |\mathcal{M}_l|^{\lambda}, \tag{51}$$

which is a very loose bound and we will provide tighter bounds in below. Before proceeding to the proof, we recall the following bounds. For $a > 1$ we have

$$\frac{1}{a-1} \leq \int_1^\infty \frac{dx}{x^a} \leq \sum_{i=1}^\infty \frac{1}{i^a} \leq 1 + \int_1^\infty \frac{dx}{x^a} = \frac{a}{a-1}, \tag{52}$$

$$\sum_{i=1}^\infty \frac{\ln(i)}{i^a} \leq \frac{\ln(2)}{2^a} + \frac{\ln(3)}{3^a} + \int_3^\infty \frac{\ln(x)dx}{x^a} = \frac{\ln(2)}{2^a} + \frac{\ln(3)}{3^a} + \frac{3^{1-a}((a-1)\ln(3)+1)}{(a-1)^2}, \tag{53}$$

$$\sum_{i=1}^\infty \frac{\ln(i)}{i^a} \geq \frac{\ln(2)}{2^a} + \int_3^\infty \frac{\ln(x)dx}{x^a} \geq \frac{\ln(2)}{2^a} + \frac{3^{1-a}((a-1)\ln(3)+1)}{(a-1)^2}. \tag{54}$$

For $a < 1$, we have

$$\frac{N^{1-a}-1}{1-a} = \int_1^N \frac{dx}{x^a} \leq \sum_{i=1}^N \frac{1}{i^a} \leq 1 + \int_1^N \frac{dx}{x^a} = \frac{N^{1-a}-a}{1-a} \leq \frac{N^{1-a}}{1-a}. \tag{55}$$

In the first case, we have

$$C_\lambda \leq \sum_{i=1}^N p_i^{1-\lambda} \leq \sum_{i=1}^N \frac{C^{1-\lambda}}{i^{\alpha(1-\lambda)}} \leq C^{1-\lambda} \frac{\alpha(1-\lambda)}{\alpha(1-\lambda)-1}, \tag{56}$$

which is bounded and independent of N. For the entropy, we notice that on $[0,1]$ the function $-p\ln p$ is non-negative, increasing on $[0, 1/e]$ and decreasing on $[1/e, 1]$.

$$H(A_S) = \sum_{i=1}^N -p_i \ln(p_i) \leq \sum_{p_i > 1/e} \frac{1}{e} + \sum_{p_i < 1/e} \frac{C}{i^\alpha} \ln \frac{i^\alpha}{C} \tag{57}$$

$$\leq 1 + \sum_{i \geq 1} \frac{C\alpha \ln i}{i^\alpha} \leq 1 + C\alpha \left(\frac{\ln(2)}{2^\alpha} + \frac{\ln(3)}{3^\alpha} + \frac{3^{1-\alpha}((\alpha-1)\ln(3)+1)}{(\alpha-1)^2} \right). \tag{58}$$

In the second case, the normalization constant Z diverges with N,

$$Z = \sum_{i=1}^N \frac{c_i}{i^\alpha} \leq \sum_{i=1}^N \frac{C}{i^\alpha} \leq C \left(1 + \int_1^N \frac{dx}{x^\alpha} \right) \leq C \left(\frac{N^{1-\alpha}}{1-\alpha} \right). \tag{59}$$

And using $c_i \geq c$, we have a lower bound for Z

$$Z \geq c \left(\int_1^N \frac{dx}{x^\alpha} \right) \geq \frac{c(N^{1-\alpha}-1)}{1-\alpha}. \tag{60}$$

Thus Z is of order $N^{1-\alpha}$, i.e. $Z = \Omega(N^{1-\alpha})$.

We recall the formula of C_λ from (14)

$$\ln C_\lambda = \ln \left(\sum_{i=1}^N p_i^{1-\lambda} \right) - \lambda H(A_S). \tag{61}$$

For the first term on the righthand side of (61), we have

$$\begin{aligned} \ln \left(\sum_{i=1}^N p_i^{1-\lambda} \right) &= \ln \left(\sum_{i=1}^N \left(\frac{c_i}{Z i^\alpha} \right)^{1-\lambda} \right) = -(1-\lambda)\ln(Z) + \ln \left(\sum_{i=1}^N \frac{c_i^{1-\lambda}}{i^{(1-\lambda)\alpha}} \right) \\ &= -(1-\lambda)\ln(N^{1-\alpha}) + \ln(N^{1-(1-\lambda)\alpha}) + \mathcal{E}_0 = \lambda \ln N + \mathcal{E}_0, \end{aligned} \tag{62}$$

where

$$|\mathcal{E}_0 - (\ln(1-(1-\lambda)\alpha) - (1-\lambda)\ln(1-\alpha))| \leq (1-\lambda)\ln(C/c) \tag{63}$$

Next we compute the entropy $H(A_S)$ and show it diverges as $\ln N$.

$$\begin{aligned} H(A_S) &= -\sum_{i=1}^{N} p_i \ln(p_i) = -\sum_{i=1}^{N} p_i \ln \frac{c_i}{i^\alpha Z} = \alpha \sum_{i=1}^{N} p_i \ln(i) + \ln(Z) - \sum_{i=1}^{N} p_i \ln(c_i) \\ &= \alpha \sum_{i=1}^{N} p_i \ln(i) + (1-\alpha)\ln N + \mathcal{E}_1, \end{aligned} \tag{64}$$

where

$$\ln(c/C) - \ln(1-\alpha) \le \mathcal{E}_1 \le \ln(C/c) - \ln(1-\alpha) \tag{65}$$

To compute the first term on the righthand side of (64), we introduce

$$S_i = \frac{c_1}{1^\alpha} + \frac{c_2}{2^\alpha} + \cdots + \frac{c_i}{i^\alpha}, \quad 1 \le i \le N, \tag{66}$$

then $S_N = Z$. Next we can do a summation by part

$$\begin{aligned} \sum_{i=1}^{N} p_i \ln(i) &= \frac{1}{Z}\sum_{i=1}^{N} \frac{c_i}{i^\alpha} \ln(i) = \frac{1}{Z}\sum_{i=1}^{N} (S_i - S_{i-1}) \ln(i) \\ &= \frac{1}{Z}\sum_{i=1}^{N-1} S_i(\ln(i) - \ln(i+1)) + \frac{S_N \ln N}{Z} \\ &= \frac{1}{Z}\sum_{i=1}^{N-1} S_i(\ln(i) - \ln(i+1)) + \ln N \end{aligned} \tag{67}$$

The same as in (59), we have $|S_i| \le C i^{1-\alpha}/(1-\alpha)$. Moreover $\ln(1+1/i) \le 1/i$. Thus the first term on the righthand side of (67) can be bounded as

$$\left| \frac{1}{Z}\sum_{i=1}^{N-1} S_i(\ln(i) - \ln(i+1)) \right| \le \frac{1}{Z}\sum_{i=1}^{N} C\left(\frac{i^{1-\alpha}}{1-\alpha}\right)\frac{1}{i} \le \frac{C}{c(1-\alpha)} \tag{68}$$

By plugging (67) and (68) into (64), we conclude the following bound on the entropy

$$H(A_S) = \ln(N) + \mathcal{E}_2. \tag{69}$$

where

$$\ln(c/C) - \ln(1-\alpha) - \frac{C}{c(1-\alpha)} \le \mathcal{E}_2 \le \ln(C/c) - \ln(1-\alpha) + \frac{C}{c(1-\alpha)} \tag{70}$$

The two estimates (62) and (69) together imply that $C_\lambda = \mathcal{E}_0 - \lambda \mathcal{E}_2$, and

$$|C_\lambda - (\ln(1-(1-\lambda)\alpha) - (1-2\lambda)\ln(1-\alpha))| \le (2-\lambda)\ln(C/c) + \frac{C}{c(1-\alpha)} \tag{71}$$

□

C EXPERIMENTAL DETAILS FOR SECTION 4.1

C.1 TRAINING

Data. The dataset was 5-way classification on 2D clustered inputs (fig. 3). Each dataset draw contained 50 training points and 250 test points.

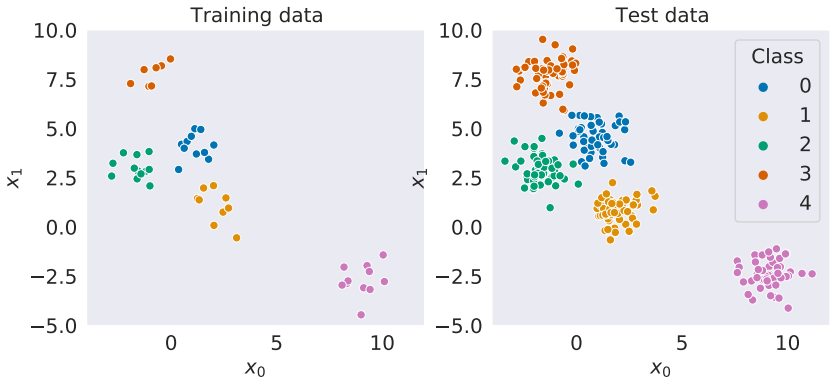


Figure 3: Example draw for 2D classification dataset.

Training. 216 models were trained for all combinations of options: 4 ReLU-activated MLP architectures (per-layer widths of [256, 256, 128, 128], [128, 128, 64, 64], [64, 64, 32, 32], [32, 32, 16, 16]), 3 weight decay rates (0, 0.01, 0.1), 3 dataset draws, 3 random seeds, and 2 sample set sizes for evaluating $I(X; Z_l^s)$ and $I(X; Z_l^s|Y)$. Final features were sampled from deterministically computed mean and standard deviation vectors and mapped to class probabilities with a softmax-activated linear layer. The expectation in MI over $\mathbb{P}(Z_l^s|x)$ depends on neural network parameters, so the reparameterization trick was used to optimize the expectation with respect to neural network parameters by rewriting the expectation over Z_l^s as an expectation over random noise (Kingma et al., 2015). Models were trained for 300 iterations with a learning rate of $\eta_\theta = 1e-2$. Out of all settings, 36 models with training set accuracy $< 85\%$ were discarded. Statistics for accepted models are given in table 4. Of 180 accepted models, 9 (5%) had a small negative generalization gap in loss (-0.0258 ± 0.0161). These models were not screened out before evaluating the metrics because the generalization gap is not estimatable without access to labelled test data.

	Mean	Standard deviation	Max	Min
Train loss	0.1265	0.1603	0.5757	0.0018
Train accuracy	0.9680	0.0479	1.0000	0.8600
Test loss	0.1984	0.1593	0.5487	0.0247
Test accuracy	0.9356	0.0568	0.9960	0.7880

Table 4: Performance statistics of 180 accepted models.

Constrained optimization. In each learning iteration, the gradient of the relaxed problem $\theta \leftarrow \theta - \eta_\theta \nabla_\theta \big[\big(-\frac{1}{|s|} \sum_{(x,y)\in s} \big(\log \frac{1}{k} \sum_{j=1}^{k} q_\theta(y|z^j) \big) \big) + \lambda(\rho - \hat{I}(X; Z_l^s))\big]$ was applied to update the model and $\lambda \leftarrow \lambda + \eta_\lambda(\rho - \hat{I}(X; Z_l^s))$ was applied to update the multiplier λ, where η_θ and η_λ are learning rates. For a similar use case for dual gradient descent, see Eysenbach et al. (2021). Example plots showing the change in $\hat{I}(X; Z_l^s)$ and λ during training are given in fig. 4. Note that the gradient of λ is a term in the gradient of θ, thus updating λ incurs negligible additional cost.

C.2 Metrics

SWAG provides an estimate of the posterior as a multivariate Gaussian by averaging gradient updates across training epochs. SWAG was used in the estimator $\breve{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) = (1/|D|) \sum_{s\in D} (1/k) \sum_{j=1}^{k} (\log p(w^j|s)) - ((1/|D|) \sum_{s'\in D} \log p(w^j|s')) \geq (1/|D|) \sum_{s\in D} (1/k) \sum_{j=1}^{k} \log(p(w^j|s)/((1/|D|) \sum_{s'\in D} p(w^j|s')))$ where $w^j \sim \mathbb{P}(\theta_l^{\mathbf{S}}|\mathbf{S} = s)$ and the upper bound is obtained via Jensen's inequality. We found that averaging in the log domain by using the upper bound improved numerical stability compared to averaging in the probability domain due to large magnitudes of $\log p(w^j|s')$.

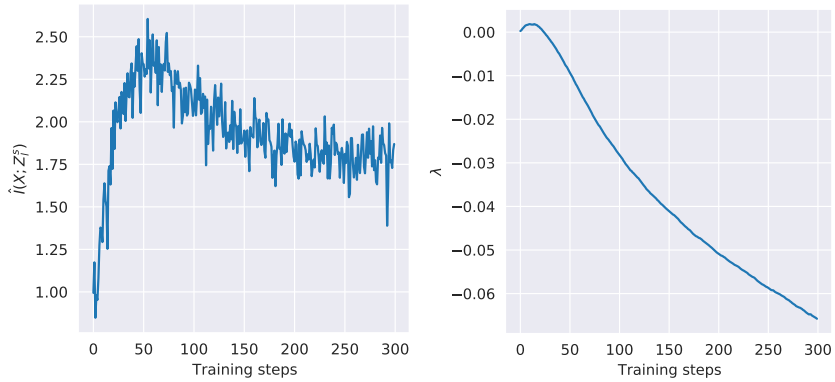


Figure 4: Example plots of $\hat{I}(X; Z_l^s)$ and λ during constrained optimized of a neural network model with $\rho = 1.5$.

Mutual information between variables is a measure of their statistical dependence and is defined in our setting as:

$$I(X; Z_l^s) = \mathbb{E}_{X, Z_l^s} \log \frac{q_\theta(Z_l^s|X)}{\mathbb{E}_{X'} q_\theta(Z_l|X')}, \tag{72}$$

$$I(X; Z_l^s|Y) = \mathbb{E}_Y \mathbb{E}_{X_Y, Z_l^s} \log \frac{q_\theta(Z_l^s|X_Y)}{\mathbb{E}_{X'_Y} q_\theta(Z_l^s|X'_Y)}, \tag{73}$$

$$I(\mathbf{S}; \theta_l^{\mathbf{S}}) = \mathbb{E}_{\mathbf{S}} \mathbb{E}_{\theta_l^{\mathbf{S}}|S} \log \frac{\mathbb{P}(\Theta|\mathbf{S})}{\mathbb{E}_{\mathbf{S}'} \mathbb{P}(\Theta|\mathbf{S}')}, \tag{74}$$

$$\tag{75}$$

where X', X'_Y, $\mathbf{S}'$ are independent copies of variables X, X_Y, $\mathbf{S}$ respectively. Let C be the set of classes and s_c denote dataset samples for class c. We use $\hat{I}$ to denote estimation by Monte-Carlo sampling and $\breve{I}$ to denote upper bounding via the Jensen inequality:

$$\hat{I}(X; Z_l^s) = \frac{1}{|s|} \sum_{(x,y)\in s} \frac{1}{k} \sum_{j=1}^{k} \log \frac{q_\theta(z^j|x)}{\frac{1}{|s|} \sum_{(x',y')\in s} q_\theta(z^j|x')}, \tag{76}$$

$$\hat{I}(X; Z_l^s|Y) = \frac{1}{|s|} \sum_{c\in C} \sum_{(x,y)\in s_c} \frac{1}{k} \sum_{j=1}^{k} \log \frac{q_\theta(z^j|x)}{\frac{1}{|s_c|} \sum_{(x',y')\in s_c} q_\theta(z^j|x')}, \tag{77}$$

$$\breve{I}(X; Z_l^s) = \frac{1}{|s|} \sum_{(x,y)\in s} \frac{1}{k} \sum_{j=1}^{k} \left(\log q_\theta(z^j|x) - \left(\frac{1}{|s|} \sum_{(x',y')\in s} \log q_\theta(z^j|x') \right) \right), \tag{78}$$

$$\breve{I}(X; Z_l^s|Y) = \frac{1}{|s|} \sum_{c\in C} \sum_{(x,y)\in s_c} \frac{1}{k} \sum_{j=1}^{k} \left(\log q_\theta(z^j|x) - \left(\frac{1}{|s_c|} \sum_{(x',y')\in s_c} \log q_\theta(z^j|x') \right) \right), \tag{79}$$

where $z^j \sim q_\theta(Z_l^s|x)$ for all j.

For mutual information between the model and training dataset, we compute:

$$\breve{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) = \frac{1}{|D|} \sum_{s\in D} \frac{1}{k} \sum_{j=1}^{k} \left(\log p(w^j|s) - \left(\frac{1}{|D|} \sum_{s'\in D} \log p(w^j|s') \right) \right), \tag{80}$$

where $w^j \sim \mathbb{P}(\theta_l^{\mathbf{S}}|\mathbf{S} = s)$. The learning algorithm is defined by the variables excluding the training dataset, i.e. architecture, weight decay, multiplier learning rate, seed. Denote the average values of

$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})$ and $\hat{I}(X;Z_l^s|Y)$ across learning algorithms by μ and μ' respectively. The rescaled value $\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}})$ is defined by:

$$\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}}) = \frac{\mu'}{\mu}\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}). \tag{81}$$

Note that MI is measured in universal units, but we test multiple estimation procedures for $I(X;Z_l^s)$ and $I(\mathbf{S};\theta_l^{\mathbf{S}})$. Scaling was tested because of the difference of estimators, rather than of units of the estimated quantity.

C.3 Additional results

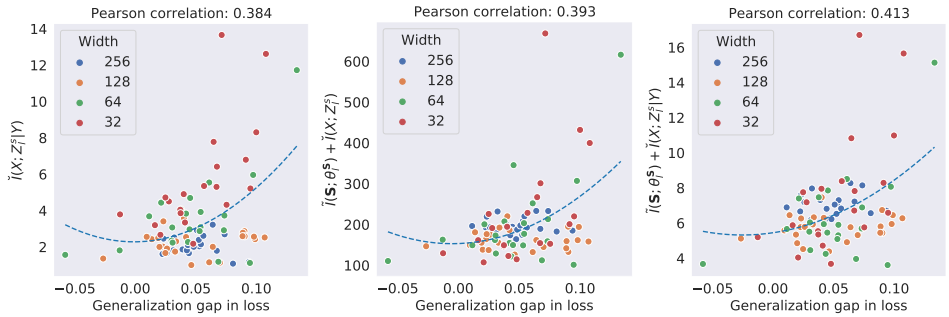
As the true data generator is available for the toy dataset, 2 sample set sizes were considered for computing estimators of $I(X;Z_l^s)$ and $I(X;Z_l^s|Y)$ during evaluation of the metrics (appendix C.1): using the training dataset (50 data points), and using a sample 10 times larger drawn from the generator (500 data points). Using the larger sample size (tables 1 and 5) improved the predictive ability of the baseline representation compression metrics compared to using the small sample size (table 6).

Metric	Spearman	Pearson	Kendall
Num. params. m	-0.0576	-0.0294	-0.0402
$m \log m$	-0.0576	-0.0287	-0.0402
$\sum_{\mathbf{l}} \theta_{\mathbf{l}}^{\mathbf{S}}$	-0.2550	-0.1366	-0.1567
$\prod_{\mathbf{l}} \theta_{\mathbf{l}}^{\mathbf{S}}$	-0.2172	-0.0871	-0.1374
$\hat{I}(X;Z_l^s)$	0.1816	0.2878	0.1280
$\hat{I}(X;Z_l^s|Y)$	0.1749	0.3167	0.1129
$\breve{I}(X;Z_l^s)$	0.1648	0.3712	0.1223
$\breve{I}(X;Z_l^s|Y)$	0.2293	0.3842	0.1515
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})$	0.0020	0.0211	0.0074
$\breve{I}(\mathbf{S};\theta_{D+1}^{\mathbf{S}})$	-0.0221	0.0091	-0.0090
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s)$	0.0178	0.0211	0.0178
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s|Y)$	0.0163	0.0211	0.0167
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s)$	0.0135	0.0212	0.0162
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s|Y)$	0.0164	0.0211	0.0167
$\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s)$	0.1104	0.1401	0.0794
$\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s|Y)$	0.2253	0.3177	0.1567
$\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s)$	0.2684	0.3928	0.1912
$\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s|Y)$	**0.3015**	**0.4130**	**0.2085**

Table 5: Correlation coefficients for metrics and the generalization gap in loss, large sample setting for estimation of $I(X;Z_l^s)$ and $I(X;Z_l^s|Y)$. $\theta_{\mathbf{l}}^{\mathbf{S}}$ denotes parameters of layer $\mathbf{l}$ and $\theta_l^{\mathbf{S}}$ denotes parameters up to layer l. Layer l is fixed to the penultimate layer. > 0 indicates positive correlation.

Metric	Spearman	Pearson	Kendall
$\hat{I}(X;Z_l^s)$	-0.1066	-0.0972	-0.0709
$\hat{I}(X;Z_l^s|Y)$	0.0868	0.0394	0.0698
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s|Y)$	0.2360	0.2489	0.1611
$\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s|Y)$	**0.3277**	**0.2888**	**0.2257**

Table 6: Correlation coefficients for metrics and the generalization gap in loss, small sample setting for estimation of $I(X;Z_l^s)$ and $I(X;Z_l^s|Y)$. Best metric and ablation shown. Layer l is fixed to the penultimate layer. > 0 indicates positive correlation.



(a) $\breve{I}(X; Z_l^s|Y)$ (b) $\tilde{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) + \breve{I}(X; Z_l^s)$ (c) $\tilde{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) + \breve{I}(X; Z_l^s|Y)$

Figure 5: Correlation of best 3 metrics with the generalization gap. Color denotes network width. Dashed line denotes best polynomial fit with degree 2.

D MNIST AND FASHION MNIST

We conducted experiments on the MNIST and Fashion MNIST datasets. These experiments follow the same protocol described in section 4.1 and appendix C except that MI was not constrained, in order to investigate predictive ability of the metrics in the setting of unconstrained stochastic feature models. 144 models were trained over all combinations of options: 2 datasets, 3 ReLU-activated architectures (1 convolutional layer and 3 linear layers, with per hidden layer channel sizes of [64, 512, 512], [32, 256, 256], [16, 128, 128]), 2 weight decay rates (0, 1e-3), 2 batch sizes (128, 32), 3 dataset draws, 2 random seeds. As in section 4.1 and appendix C, the penultimate layer of the network infers mean and standard deviation vectors that define a distribution over latent features. To construct multiple instances of the training dataset, we sampled training datasets of size 8K from the training set, and each test set was the original 10K test set. Performance of trained models are given in tables 9 and 10. In line with sections 4.1 and 4.2 and appendices C and E, results on MNIST and Fashion MNIST indicate that metrics which combine model compression with representation compression outperform metrics for representation compression alone (tables 7 and 8).

Metric	Spearman	Pearson	Kendall
$\hat{I}(X; Z_l^s)$	0.2738	-0.1268	0.2178
$\hat{I}(X; Z_l^s\|Y)$	0.4399	0.2059	0.3243
$\breve{I}(X; Z_l^s)$	0.7895	0.5467	0.6346
$\breve{I}(X; Z_l^s\|Y)$	0.7931	0.5348	**0.6416**
$\breve{I}(\mathbf{S}; \theta_l^{\mathbf{S}})$	0.6004	0.7044	0.4193
$\bar{I}(\mathbf{S}; \theta_l^{\mathbf{S}})$	0.5328	0.6906	0.3771
$\breve{I}(\mathbf{S}; \theta_{D+1}^{\mathbf{S}})$	0.5384	0.6619	0.3768
$\bar{I}(\mathbf{S}; \theta_{D+1}^{\mathbf{S}})$	0.5328	0.6507	0.3771
$\tilde{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) + \hat{I}(X; Z_l^s)$	0.6021	0.7043	0.4130
$\tilde{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) + \hat{I}(X; Z_l^s\|Y)$	0.5958	0.7044	0.3955
$\tilde{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) + \breve{I}(X; Z_l^s)$	**0.8352**	0.6367	**0.6452**
$\tilde{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) + \breve{I}(X; Z_l^s\|Y)$	**0.8303**	0.6242	0.6384
$\breve{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) + \hat{I}(X; Z_l^s)$	0.6021	0.7044	0.4130
$\breve{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) + \hat{I}(X; Z_l^s\|Y)$	0.5958	0.7044	0.3955
$\breve{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) + \breve{I}(X; Z_l^s)$	0.7128	**0.7626**	0.5119
$\breve{I}(\mathbf{S}; \theta_l^{\mathbf{S}}) + \breve{I}(X; Z_l^s\|Y)$	0.6566	**0.7329**	0.4610

Table 7: MNIST. Correlation coefficients for metrics and the generalization gap in loss. Layer l is fixed to the penultimate layer. > 0 indicates positive correlation.

Metric	Spearman	Pearson	Kendall
$\hat{I}(X;Z_l^s)$	-0.0299	-0.2056	-0.0261
$\hat{I}(X;Z_l^s\|Y)$	0.2318	0.1185	0.1458
$\breve{I}(X;Z_l^s)$	0.3861	0.5146	0.2293
$\breve{I}(X;Z_l^s\|Y)$	0.3848	0.5115	0.2308
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})$	0.3479	0.3191	0.2682
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})$	0.3471	0.2804	0.2684
$\breve{I}(\mathbf{S};\theta_{D+1}^{\mathbf{S}})$	0.3479	0.3187	0.2682
$\bar{I}(\mathbf{S};\theta_{D+1}^{\mathbf{S}})$	0.3928	0.3121	0.2998
$\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s)$	0.3377	0.3188	0.2469
$\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s\|Y)$	0.3446	0.3191	0.2660
$\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s)$	**0.5623**	**0.6488**	**0.4238**
$\tilde{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s\|Y)$	**0.5637**	**0.6441**	**0.4344**
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s)$	0.3377	0.3191	0.2469
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s\|Y)$	0.3446	0.3191	0.2660
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s)$	0.3734	0.3280	0.2677
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s\|Y)$	0.3679	0.3217	0.2766

Table 8: Fashion MNIST. Correlation coefficients for metrics and the generalization gap in loss. Layer l is fixed to the penultimate layer. > 0 indicates positive correlation.

	Mean	Standard deviation	Max	Min
Train loss	0.0071	0.0165	0.1053	0.0001
Train accuracy	0.9986	0.0060	1.0000	0.9628
Test loss	0.1355	0.0285	0.2564	0.0915
Test accuracy	0.9673	0.0065	0.9737	0.9358

Table 9: Performance statistics for MNIST models.

	Mean	Standard deviation	Max	Min
Train loss	0.0692	0.0640	0.1908	0.0003
Train accuracy	0.9765	0.0234	1.0000	0.9329
Test loss	0.5609	0.1682	0.8819	0.3791
Test accuracy	0.8721	0.0090	0.8864	0.8262

Table 10: Performance statistics for Fashion MNIST models.

E EXPERIMENTAL DETAILS FOR SECTION 4.2

E.1 TRAINING

540 models were trained for all combinations of the options: 3 architecutres (PreResNet56, PreResNet83, PreResNet110), 3 weight decay rates (1e-3, 1e-4, 1e-5), 3 batch sizes (64, 128, 1024), 5 dataset draws and 4 random seeds. The PreResNet architecture (He et al., 2016) consists of a convolutional layer, 3 residual blocks and a final linear prediction layer. We consider representations from $D = 5$ layers: input layer, after convolutional layer, and after each residual block. Models were trained for 200 epochs with SGD and a learning rate of $1e-2$. Statistics are given in table 11.

	Mean	Standard deviation	Max	Min
Train loss	0.2157	0.2815	1.4174	0.0005
Train accuracy	0.9282	0.0937	1.0000	0.5433
Test loss	0.9704	0.2023	1.6269	0.5989
Test accuracy	0.8043	0.0554	0.8770	0.5192

Table 11: Performance statistics of 540 models.

E.2 METRICS

We used the same metrics as defined in appendix C.2 and additionally test excluding the seed from the definition of the learning algorithm by averaging across seeds. Let G denote the set of seeds and let Γ denote the seed variable:

$$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) = \frac{1}{|D||G|}\sum_{s\in D}\sum_{\gamma\in G}\frac{1}{k}\sum_{j=1}^{k}\left(\left(\frac{1}{|G|}\sum_{\gamma'\in G}\log p(w^j|s,\gamma')\right) - \left(\frac{1}{|D||G|}\sum_{s'\in D}\sum_{\gamma'\in G}\log p(w^j|s',\gamma')\right)\right) \tag{82}$$

where $w^j \sim \mathbb{P}(\theta_l^{\mathbf{S}}|\mathbf{S}=s,\Gamma=\gamma)$ is sampled from the estimated posterior produced by SWAG.

E.3 KERNEL DENSITY ESTIMATION

Without the addition of noise in the hidden representation, mutual information between inputs and deterministic continuous features is ill-defined (Saxe et al., 2019). One way to add noise is to discretize hidden activity into bins (Shwartz-Ziv & Tishby, 2017). Another approach is kernal density estimation (Kolchinsky & Tracey, 2017), which assumes for the purpose of analysis that Gaussian noise with variance σ_l^2 is added to the representation produced by layer l. In adaptive KDE (Chelombiev et al., 2019) σ_l^2 is scaled from a base by the maximum observed activation level in the layer, improving on constant σ_l^2 (Saxe et al., 2019) by allowing the level of noise to vary with layers. Following the previous work, we found $1e-3$ to work well as the base value.

As an alternative method for specifying σ_l^2, we selected σ_l^2 from a discrete set by maximum log likelihood of observed features,

$$\frac{1}{|s|}\sum_{(x,y)\in s}\frac{1}{k}\sum_{j=1}^{k}\log\frac{1}{|s|}\sum_{(x',y')\in s}q_\theta(z^j|x') \qquad \text{where } z^j\sim q_\theta(Z_l^s|x), \tag{83}$$

under the constraint that estimated MI decreased with layer, which follows from the information processing inequality. This was performed by iterating from layer D to layer 1 and choosing σ_l^2 with maximum likelihood such that the estimator of MI was non-decreasing, i.e. $\hat{I}(X;Z_l^s)\geq\hat{I}(X;Z_{l+1}^s)$ for $l<D$. As with estimators in appendix C.2, averaging can be done in the log domain to yield the lower bound:

$$\frac{1}{|s|}\sum_{(x,y)\in s}\frac{1}{k}\sum_{j=1}^{k}\frac{1}{|s|}\sum_{(x',y')\in s}\log q_\theta(z^j|x') \qquad \text{where } z^j\sim q_\theta(Z_l^s|x). \tag{84}$$

For consistency, eq. (83) was used with $\hat{I}(X; Z_l^s)$ (eq. (76)) and eq. (84) with $\breve{I}(X; Z_l^s)$ (eq. (78)).

E.4 FURTHER RESULTS

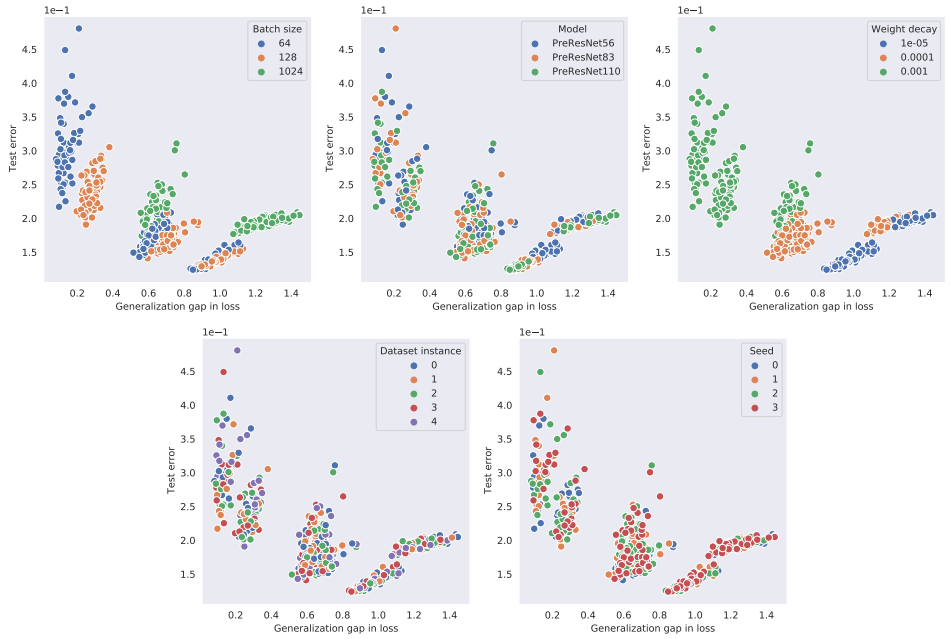


Figure 6: Illustration of performance-based clustering behaviour that emerged from training, attributed mostly to batch size and weight decay.

	Spearman corr.		Pearson corr.		Kendall corr.	
Generalization gap:	Loss	Error	Loss	Error	Loss	Error
Train loss	-0.8075	-0.7229	-0.8376	-0.8730	-0.5632	-0.5307
Test loss	0.6970	0.6095	0.6497	0.5210	0.5938	0.4777
Train error	-0.8114	-0.7269	-0.8489	-0.8831	-0.5707	-0.5381
Test error	-0.4609	-0.3834	-0.5896	-0.6087	-0.2652	-0.2020
Gen. gap error	0.9443	1.0000	0.9562	1.0000	0.8149	1.0000
Gen. gap loss	1.0000	0.9443	1.0000	0.9562	1.0000	0.8149

Table 12: Results for prediction with performance metrics.

Layer index l:	1	2	3	4	5
$\breve{I}(X;Z_l^s)$	5.9422E+04	1.8236E+04	1.5514E+04	7.7865E+03	5.7027E+03
$\breve{I}(X;Z_l^s\|Y)$	5.7783E+04	1.7790E+04	1.5429E+04	7.6948E+03	5.3298E+03
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})$	0.0000E+00	3.7136E+03	9.4890E+05	2.1247E+06	5.8244E+06
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s\|Y)$	5.7783E+04	2.1504E+04	9.6433E+05	2.1324E+06	5.8297E+06

Table 13: Example values of metrics, for best performing model by test loss (PreResNet56, batch size 128, weight decay 0.001). $l = 1$ is the input layer.

	Spearman corr.		Pearson corr.		Kendall corr.	
Generalization gap:	Loss	Error	Loss	Error	Loss	Error
$\breve{I}(S;\theta_{D+1}^{\mathbf{S}})$	0.4688	0.3112	0.2512	0.0775	0.2121	0.1208
$\bar{I}(S;\theta_{D+1}^{\mathbf{S}})$	0.5370	0.3800	0.2924	0.1218	0.2442	0.1526

Table 14: Results for model compression metrics.

	Layer	Spearman corr.		Pearson corr.		Kendall corr.	
Generalization gap:		Loss	Error	Loss	Error	Loss	Error
$\hat{I}(X;Z_l^s)$	$l = 1$	0.7345	0.6156	0.5722	0.3853	0.5174	0.4215
$\hat{I}(X;Z_l^s)$	$l = D$	0.7170	0.5740	0.7063	0.5602	0.4784	0.3721
$\hat{I}(X;Z_l^s\|Y)$	$l = 1$	0.7199	0.6073	0.5724	0.3854	0.5005	0.4111
$\hat{I}(X;Z_l^s\|Y)$	$l = D$	0.7126	0.5691	0.7071	0.5616	0.4768	0.3700
$\breve{I}(X;Z_l^s)$	$l = 1$	0.6765	0.5655	0.1554	0.1328	0.4553	0.3781
$\breve{I}(X;Z_l^s)$	$l = D$	0.7145	0.5602	0.7203	0.5719	0.4461	0.3404
$\breve{I}(X;Z_l^s\|Y)$	$l = 1$	0.6476	0.5292	0.1557	0.1331	0.4307	0.3504
$\breve{I}(X;Z_l^s\|Y)$	$l = D$	0.7004	0.5434	0.7062	0.5560	0.4386	0.3305

Table 15: Results for representation compression metrics for $l \in \{1, D\}$ summarization over layers (MLE selection of σ_l^2).

	Layer	Spearman corr.		Pearson corr.		Kendall corr.	
Generalization gap:		Loss	Error	Loss	Error	Loss	Error
$\hat{I}(X;Z_l^s)$	$l = 1$	-0.0681	-0.0659	-0.0645	-0.0617	-0.0464	-0.0447
$\hat{I}(X;Z_l^s)$	$l = D$	0.7019	0.5452	0.4596	0.2845	0.4329	0.3293
$\hat{I}(X;Z_l^s\|Y)$	$l = 1$	0.0050	0.0032	0.0146	0.0191	0.0035	0.0022
$\hat{I}(X;Z_l^s\|Y)$	$l = D$	0.6977	0.5403	0.4544	0.2798	0.4302	0.3268
$\breve{I}(X;Z_l^s)$	$l = 1$	-0.0196	-0.0080	-0.0070	-0.0029	-0.0139	-0.0051
$\breve{I}(X;Z_l^s)$	$l = D$	0.7314	0.5848	0.5109	0.3350	0.4645	0.3624
$\breve{I}(X;Z_l^s\|Y)$	$l = 1$	0.0005	-0.0060	0.0036	-0.0001	0.0005	-0.0038
$\breve{I}(X;Z_l^s\|Y)$	$l = D$	0.7033	0.5465	0.4587	0.2846	0.4342	0.3304

Table 16: Results for metrics for $l \in \{1, D\}$ summarization over layers (adaptive KDE selection of σ_l^2).

Generalization gap:	Layer	Spearman corr. Loss	Spearman corr. Error	Pearson corr. Loss	Pearson corr. Error	Kendall corr. Loss	Kendall corr. Error
$\hat{I}(X;Z_l^s)$	Mean	0.7598	0.6184	0.5781	0.3911	0.4970	0.3936
$\hat{I}(X;Z_l^s)$	Max	0.7345	0.6156	0.5722	0.3853	0.5174	0.4215
$\hat{I}(X;Z_l^s)$	Min	0.7170	0.5740	0.7063	0.5602	0.4784	0.3721
$\hat{I}(X;Z_l^s\|Y)$	Mean	0.7720	0.6378	0.5790	0.3920	0.5186	0.4145
$\hat{I}(X;Z_l^s\|Y)$	Max	0.7049	0.5814	0.5723	0.3853	0.4712	0.3785
$\hat{I}(X;Z_l^s\|Y)$	Min	0.7137	0.5701	0.7112	0.5679	0.4775	0.3697
$\breve{I}(X;Z_l^s)$	Mean	0.8481	0.7410	0.2116	0.1831	0.6425	0.5436
$\breve{I}(X;Z_l^s)$	Max	0.6765	0.5655	0.1554	0.1328	0.4553	0.3781
$\breve{I}(X;Z_l^s)$	Min	0.7145	0.5602	0.7203	0.5719	0.4461	0.3404
$\breve{I}(X;Z_l^s\|Y)$	Mean	0.8481	0.7406	0.2140	0.1853	0.6427	0.5435
$\breve{I}(X;Z_l^s\|Y)$	Max	0.6486	0.5297	0.1557	0.1331	0.4316	0.3511
$\breve{I}(X;Z_l^s\|Y)$	Min	0.7004	0.5434	0.7062	0.5560	0.4386	0.3305
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s)$	Mean	0.4546	0.3055	0.1867	0.0160	0.2304	0.1398
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s)$	Max	0.5111	0.3609	0.2572	0.0858	0.2634	0.1715
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s)$	Min	0.8134	0.6906	0.5363	0.3729	0.5840	0.4870
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s\|Y)$	Mean	0.4543	0.3052	0.1858	0.0152	0.2305	0.1397
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s\|Y)$	Max	0.5112	0.3609	0.2572	0.0858	0.2637	0.1718
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s\|Y)$	Min	0.8136	0.6949	0.5193	0.3591	0.5817	0.4871
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s)$	Mean	0.4513	0.3026	0.1832	0.0132	0.2305	0.1398
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s)$	Max	0.5112	0.3609	0.2572	0.0858	0.2636	0.1715
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s)$	Min	0.8489	0.7353	0.8459	0.7216	0.6354	0.5386
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s\|Y)$	Mean	0.4513	0.3026	0.1832	0.0132	0.2301	0.1397
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s\|Y)$	Max	0.5113	0.3609	0.2572	0.0858	0.2638	0.1716
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s\|Y)$	Min	0.8434	0.7313	0.8437	0.7195	0.6270	0.5332
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s)$	Mean	0.4770	0.3244	0.2901	0.1155	0.2510	0.1568
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s)$	Max	0.5709	0.4205	0.2993	0.1311	0.2878	0.1946
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s)$	Min	0.7898	0.6548	0.6706	0.4929	0.5432	0.4412
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s\|Y)$	Mean	0.4764	0.3241	0.2869	0.1128	0.2489	0.1558
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s\|Y)$	Max	0.5709	0.4205	0.2993	0.1311	0.2882	0.1952
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\hat{I}(X;Z_l^s\|Y)$	Min	0.7917	0.6595	0.6490	0.4753	0.5447	0.4450
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s)$	Mean	0.4429	0.2910	0.2785	0.1060	0.2353	0.1432
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s)$	Max	0.5707	0.4205	0.2993	0.1311	0.2880	0.1946
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s)$	Min	**0.8635**	**0.7576**	**0.8493**	**0.7544**	**0.6660**	**0.5684**
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s\|Y)$	Mean	0.4429	0.2908	0.2783	0.1059	0.2349	0.1426
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s\|Y)$	Max	0.5711	0.4204	0.2993	0.1311	0.2886	0.1945
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}})+\breve{I}(X;Z_l^s\|Y)$	Min	**0.8632**	**0.7576**	**0.8511**	**0.7562**	**0.6626**	**0.5664**

Table 17: Results for metrics for mean, min, max summarization over layers (MLE selection of σ_l^2). Best metrics highlighted.

Generalization gap:	Layer	Spearman corr. Loss	Spearman corr. Error	Pearson corr. Loss	Pearson corr. Error	Kendall corr. Loss	Kendall corr. Error
$\hat{I}(X;Z_l^s)$	Mean	0.7322	0.5837	0.6823	0.5067	0.4606	0.3605
$\hat{I}(X;Z_l^s)$	Max	0.7805	0.6521	0.6848	0.5088	0.5299	0.4360
$\hat{I}(X;Z_l^s)$	Min	0.7726	0.6450	0.8131	0.7004	0.5126	0.4205
$\hat{I}(X;Z_l^s\|Y)$	Mean	0.7323	0.5833	0.6863	0.5110	0.4604	0.3598
$\hat{I}(X;Z_l^s\|Y)$	Max	0.7865	0.6548	0.6920	0.5160	0.5378	0.4380
$\hat{I}(X;Z_l^s\|Y)$	Min	0.7731	0.6451	0.8175	0.7041	0.5131	0.4221
$\breve{I}(X;Z_l^s)$	Mean	0.7401	0.5933	0.7078	0.5334	0.4739	0.3727
$\breve{I}(X;Z_l^s)$	Max	0.7452	0.6264	0.6891	0.5116	0.4927	0.4109
$\breve{I}(X;Z_l^s)$	Min	0.7981	0.6720	**0.8515**	**0.7262**	0.5490	0.4500
$\breve{I}(X;Z_l^s\|Y)$	Mean	0.7375	0.5894	0.7010	0.5263	0.4701	0.3685
$\breve{I}(X;Z_l^s\|Y)$	Max	0.7449	0.6177	0.7056	0.5289	0.4924	0.4053
$\breve{I}(X;Z_l^s\|Y)$	Min	0.7686	0.6270	0.8130	0.6699	0.5093	0.4055
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s)$	Mean	0.4555	0.3070	0.1856	0.0153	0.2334	0.1425
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s)$	Max	0.5133	0.3633	0.2580	0.0865	0.2650	0.1735
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s)$	Min	0.8112	0.7033	0.8272	0.7243	0.5775	0.4914
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s\|Y)$	Mean	0.4542	0.3058	0.1849	0.0146	0.2322	0.1414
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s\|Y)$	Max	0.5126	0.3625	0.2578	0.0863	0.2643	0.1730
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s\|Y)$	Min	**0.8205**	**0.7203**	0.8281	**0.7313**	**0.5913**	**0.5108**
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s)$	Mean	0.4602	0.3115	0.1878	0.0172	0.2378	0.1468
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s)$	Max	0.5146	0.3647	0.2588	0.0871	0.2666	0.1748
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s)$	Min	0.8014	0.6854	0.8423	0.7107	0.5658	0.4760
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s\|Y)$	Mean	0.4598	0.3111	0.1874	0.0168	0.2374	0.1464
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s\|Y)$	Max	0.5143	0.3643	0.2584	0.0868	0.2661	0.1743
$\breve{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s\|Y)$	Min	0.8069	0.6913	**0.8440**	0.7135	0.5732	0.4849
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s)$	Mean	0.4783	0.3249	0.2868	0.1134	0.2495	0.1577
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s)$	Max	0.5765	0.4250	0.3021	0.1333	0.2971	0.2057
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s)$	Min	0.8031	0.6920	0.8270	0.7149	0.5664	0.4793
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s\|Y)$	Mean	0.4766	0.3242	0.2842	0.1110	0.2468	0.1551
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s\|Y)$	Max	0.5759	0.4247	0.3013	0.1326	0.2958	0.2049
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \hat{I}(X;Z_l^s\|Y)$	Min	**0.8130**	**0.7070**	0.8295	0.7203	**0.5799**	**0.4963**
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s)$	Mean	0.4864	0.3335	0.2946	0.1205	0.2613	0.1689
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s)$	Max	0.5769	0.4253	0.3048	0.1356	0.2978	0.2067
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s)$	Min	0.7974	0.6749	0.8206	0.6842	0.5608	0.4684
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s\|Y)$	Mean	0.4851	0.3317	0.2933	0.1192	0.2596	0.1674
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s\|Y)$	Max	0.5770	0.4253	0.3034	0.1343	0.2981	0.2068
$\bar{I}(\mathbf{S};\theta_l^{\mathbf{S}}) + \breve{I}(X;Z_l^s\|Y)$	Min	0.7989	0.6763	0.8242	0.6891	0.5628	0.4703

Table 18: Results for metrics for mean, min, max summarization over layers (adaptive KDE selection of σ_l^2). Best metrics highlighted.