Learnability for the Information Bottleneck

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Abstract

The Information Bottleneck (IB) method (Tishby et al. (2000)) provides an insightful and principled approach for balancing compression and prediction for representation learning. The IB objective $I(X;Z) - \beta I(Y;Z)$ employs a Lagrange multiplier $\beta$ to tune this trade-off. However, in practice, not only is $\beta$ chosen empirically without theoretical guidance, there is also a lack of theoretical understanding between $\beta$, learnability, the intrinsic nature of the dataset and model capacity. In this paper, we show that if $\beta$ is improperly chosen, learning cannot happen – the trivial representation $P(Z|X) = P(Z)$ becomes the global minimum of the IB objective. We show how this can be avoided, by identifying a sharp phase transition between the unlearnable and the learnable which arises as $\beta$ is varied. This phase transition defines the concept of IB-Learnability. We prove several sufficient conditions for IB-Learnability, which provides theoretical guidance for choosing a good $\beta$.

We further show that IB-learnability is determined by the largest confident, typical, and imbalanced subset of the examples (the conspicuous subset), and discuss its relation with model capacity. We give practical algorithms to estimate the minimum $\beta$ for a given dataset. We also empirically demonstrate our theoretical conditions with analyses of synthetic datasets, MNIST, and CIFAR10.

1 INTRODUCTION

Tishby et al. (2000) introduced the Information Bottleneck (IB) objective function which learns a representation $Z$ of observed variables $(X,Y)$ that retains as little information about $X$ as possible, but simultaneously captures as much information about $Y$ as possible:

$$\min IB_\beta(X,Y;Z) = \min [I(X;Z) - \beta I(Y;Z)] \quad (1)$$

$I(\cdot)$ is the mutual information. The hyperparameter $\beta$ controls the trade-off between compression and prediction, in the same spirit as Rate-Distortion Theory (Shannon, 1948), but with a learned representation function $P(Z|X)$ that automatically captures some part of the “semantically meaningful” information, where the semantics are determined by the observed relationship between $X$ and $Y$.

The IB framework has been extended to and extensively studied in a variety of scenarios, including Gaussian variables (Chechik et al. (2005)), meta-Gaussians (Key and Roth (2012)), continuous variables via variational methods (Alemi et al. (2016); Chalk et al. (2016); Fischer (2018)), deterministic scenarios (Strouse and Schwab (2017a); Kolchinsky et al. (2019)), geometric clustering (Strouse and Schwab (2017b)), and is used for learning invariant and disentangled representations in deep neural nets (Achille and Soatto (2018a,b)). However, a core issue remains: how should we set a good $\beta$? In the original work, the authors recommend sweeping $\beta \gg 1$, which can be prohibitively expensive in practice, but also leaves open interesting theoretical questions around the relationship between $\beta$, $P(Z|X)$, and the observed data, $P(X,Y)$.

This work begins to answer some of those questions by characterizing the onset of learning. Specifically:

- We show that improperly chosen $\beta$ may result in a failure to learn: the trivial solution $P(Z|X) = P(Z)$ becomes the global minimum of the IB objective, even for $\beta \gg 1$ (Section 1.1).
- We introduce the concept of IB-Learnability, and show that when we vary $\beta$, the IB objective will un-
dernour a phase transition from the inability to learn to the ability to learn (Section 3).

- Using the second-order variation, we derive sufficient conditions for IB-Learnability, which provide theoretical guidance for choosing a good $\beta$ (Section 4).

- We show that IB-Learnability is determined by the largest confident, typical, and imbalanced subset of the examples (the conspicuous subset), reveal its relationship with the slope of the Pareto frontier at the origin on the information plane $I(X; Z)$ vs. $I(Y; Z)$, and discuss its relation to model capacity (Section 5).

- We additionally prove a deep relationship between IB-Learnability, the hypercontractivity coefficient, the contraction coefficient, and the maximum correlation (Section 5).

We also present an algorithm for estimating the onset of IB-Learnability and the conspicuous subset, and demonstrate that it does a good job of approximating both the theoretical predictions and the empirical results (Section 6). Finally, we use our main results to demonstrate on synthetic datasets, MNIST (LeCun et al., 1998) and CIFAR10 (Krizhevsky and Hinton, 2009) that the theoretical prediction for IB-Learnability closely matches experiment (Section 7).

1.1 A Motivating Example

How can we choose a good $\beta$? To gain intuition, consider learning multiple Variational Information Bottleneck (VIB) representations (Alemi et al., 2016) of MNIST (LeCun et al., 1998) at different $\beta$. We select the digits 0 and 1 for binary classification, and add class-conditional noise (Angluin and Laird, 1988) to the labels with flip probability 0.2, which simulates a general scenario where the data may be noisy and the dependence of $Y$ on $X$ is not deterministic. The algorithm only sees the corrupted labels. Fig. 1 shows the converged accuracy on the true labels for the VIB models plotted against $\beta$. We see clearly that when $\beta < 3.25$, no learning happens, and the accuracy is the same as random guessing. Beginning with $\beta > 3.25$, there is a clear phase transition where the accuracy sharply increases, indicating the objective is able to learn a non-trivial representation. This kind of phase transition is typical in our experiments in Section 7. When the noise rate is high, the transition can happen at $\beta \sim 500$; i.e., we need a large “$\beta$ force” to extract relevant information from $X$ to predict $Y$. In that case, an improperly-chosen $\beta$ in the unlearnable region will preclude learning a useful representation.

Figure 1: Accuracy for binary classification of MNIST digits 0 and 1 with 20% label noise and varying $\beta$. No learning happens for models trained at $\beta < 3.25$.

2 RELATED WORK

The original IB work (Tishby et al., 2000) provides a tabular method for exactly computing the optimal encoder distribution $P(Z|X)$ for a given $\beta$ and cardinality of the discrete representation, $|Z|$. Thus, the search for the desired model involves not only sweeping $\beta$, but also considering different representation dimensionalities. These restrictions were lifted somewhat by Chechik et al. (2005), which presents the Gaussian Information Bottleneck (GIB) for learning a multivariate Gaussian representation $Z$ of $(X, Y)$, assuming that both $X$ and $Y$ are also multivariate Gaussians. They also note the presence of the trivial solution not only when $\beta \leq 1$, but also depending on the eigenspectrum of the observed variables. However, the restriction to multivariate Gaussian datasets limits the generality of the analysis. Another analytic treatment of IB is given in Key and Roth (2012), which reformulates the objective in terms of the copula functions. As with the GIB approach, this formulation restricts the form of the data distributions – the copula functions for the joint distribution $(X, Y)$ are assumed to be known, which is unlikely in practice.

Strouse and Schwab (2017a) presents the Deterministic Information Bottleneck (DIB), which minimizes the coding cost of the representation, $H(Z)$, rather than the transmission cost, $I(X; Z)$ as in IB. This approach learns hard clusterings with different code entropies that vary with $\beta$. In this case, it is clear that a hard clustering with minimal $H(Z)$ will result in a single cluster for all of the data, which is the DIB trivial solution. No analysis is given beyond this fact to predict the actual onset of learnability, however.

The first amortized IB objective is in the Variational
Our work is also closely related to the hypercontrac-
tivity coefficient \cite{Anantharam2013,Polanyi2017}, defined as $\sup_{Z \rightarrow X \rightarrow Y} \beta_{(Y|Z)}$, which by definition equals the inverse of $\beta_{0}$, our IB-
learnability threshold. In \cite{Anantharam2013}, the authors prove that the hypercontractivity coefficient equals the contraction coefficient $\eta_{\text{KL}}(P_{Y|X}, P_{X})$, and \cite{Kim2017} propose a practical algorithm to es-
timate $\eta_{\text{KL}}(P_{Y|X}, P_{X})$, which provides a measure for potential influence in the data. Although our goal is
different, the sufficient conditions we provide for IB-
Learnability are also lower bounds for the hypercontrac-
tivity coefficient.

3 IB-LEARNABILITY

We are given instances of $(x, y) \in \mathcal{X} \times \mathcal{Y}$ drawn from a distribution with probability (density) $P(X, Y)$, where unless otherwise stated, both $X$ and $Y$ can be discrete or continuous variables. $(X, Y)$ is our training data, and may be characterized by different types of noise. The nature of this training data and the choice of $\beta$ will be suf-
cient to predict the transition from unlearnable to learn-
able.

We can learn a representation $Z$ of $X$ with conditional probability\footnote{We use capital letters $X, Y, Z$ for random variables and lowercase $x, y, z$ to denote the instance of variables, with $P(\cdot)$ and $p(\cdot)$ denoting their probability or probability density, re-
respectively.} $P(z|x)$, such that $X, Y, Z$ obey the Markov chain $Z \leftarrow X \leftrightarrow Y$. Eq. \ref{eq:ib} above gives the IB objec-
tive with Lagrange multiplier $\beta$, $\text{IB}_{\beta}(X; Y; Z)$, which is a functional of $p(z|x)$: $\text{IB}_{\beta}(X, Y; Z) = \text{IB}_{\beta}[p(z|x)]$. The IB learning task is to find a conditional probability $p(z|x)$ that minimizes $\text{IB}_{\beta}(X, Y; Z)$. The larger $\beta$, the more the objective favors making a good prediction for $Y$. Conversely, the smaller $\beta$, the more the objective favors learning a concise representation.

How can we select $\beta$ such that the IB objective learns a useful representation? In practice, the selection of $\beta$ is done empirically. Indeed, \cite{Tishby2000} recommends “sweeping $\beta$”. In this paper, we provide theoretical guidance for choosing $\beta$ by introducing the concept of IB-Learnability and providing a series of IB-learnable conditions.

Definition 1. $(X, Y)$ is $\text{IB}_{\beta}$-learnable if there exists a $Z$ given by some $p_{1}(z|x)$, such that $\text{IB}_{\beta}(X, Y; Z)|_{p_{1}(z|x)} < \text{IB}_{\beta}(X, Y; Z)|_{p(z|x) = p(z)}$, where $p(z|x) = p(z)$ character-
izes the trivial representation where $Z = Z_{\text{trivial}}$ is independent of $X$.

If $(X, Y)$ is $\text{IB}_{\beta}$-learnable, then when $\text{IB}_{\beta}(X, Y; Z)$ is globally minimized, it will not learn a trivial representa-
tion. On the other hand, if $(X, Y)$ is not $\text{IB}_{\beta}$-learnable,
then when $IB_β(X, Y; Z)$ is globally minimized, it may learn a trivial representation.

**Trivial solutions.** Definition 1 defines trivial solutions in terms of representations where $I(X; Z) = I(Y; Z) = 0$. Another type of trivial solution occurs when $I(X; Z) > 0$ but $I(Y; Z) = 0$. This type of trivial solution is not directly achievable by the IB objective, as $I(X; Z)$ is minimized, but it can be achieved by construction or by chance. It is possible that starting learning from $I(X; Z) > 0$, $I(Y; Z) = 0$ could result in access to non-trivial solutions not available from $I(X; Z) = 0$. We do not attempt to investigate this type of trivial solution in this work.

**Necessary condition for IB-Learnability.** From Definition 1 we can see that $IB_β$-Learnability for any dataset $(X; Y)$ requires $β > 1$. In fact, from the Markov chain $Z ← X ↔ Y$, we have $I(Y; Z) ≤ I(X; Z)$ via the data-processing inequality. If $β ≤ 1$, then since $I(X; Z) ≥ 0$ and $I(Y; Z) ≥ 0$, we have that $\min(I(X; Z) − βI(Y; Z)) = 0 = IB_β(X, Y; Z_{trivial})$. Hence $(X, Y)$ is not $IB_β$-learnable for $β ≤ 1$.

Due to the reparameterization invariance of mutual information, we have the following theorem for $IB_β$-Learnability:

**Theorem 1.** Let $X' = g(X)$ be an invertible map (if $X$ is a continuous variable, $g$ is additionally required to be continuous). Then $(X, Y)$ and $(X', Y)$ have the same $IB_β$-Learnability.

The proof for Theorem 1 is in Appendix B. Theorem 1 implies a favorable property for any condition for $IB_β$-Learnability: the condition should be invariant to invertible mappings of $X$. We will inspect this invariance in the conditions we derive in the following sections.

### 4 SUFFICIENT CONDITIONS FOR IB-LEARNABILITY

Given $(X, Y)$, how can we determine whether it is $IB_β$-learnable? To answer this question, we derive a series of sufficient conditions for $IB_β$-Learnability, starting from its definition. The conditions are in increasing order of practicality, while sacrificing as little generality as possible.

Firstly, Theorem 2 characterizes the $IB_β$-Learnability range for $β$, with proof in Appendix C.

**Theorem 2.** If $(X, Y)$ is $IB_{β_1}$-learnable, then for any $β_2 > β_1$, it is $IB_{β_2}$-learnable.

Based on Theorem 2, the range of $β$ such that $(X, Y)$ is $IB_β$-learnable has the form $β ∈ (β_0, +∞)$. Thus, $β_0$ is the threshold of $IB$-Learnability.

**Lemma 2.1.** $p(z|x) = p(z)$ is a stationary solution for $IB_β(X, Y; Z)$.

The proof in Appendix E shows that both first-order variations $δI(X; Z) = 0$ and $δI(Y; Z) = 0$ vanish at the trivial representation $p(z|x) = p(z)$, so $δIB_β[p(z|x)] = 0$ at the trivial representation.

Lemma 2.1 yields our strategy for finding sufficient conditions for learnability: find conditions such that $p(z|x) = p(z)$ is not a local minimum for the functional $IB_β[p(z|x)]$. Based on the necessary condition for the minimum (Appendix D), we have the following theorem.

**Theorem 3 (Suff. Cond. 1).** A sufficient condition for $(X, Y)$ to be $IB_β$-learnable is that there exists a perturbation function $h(z|x)$ with $h(z|x)dz = 0$, such that the second-order variation $δ^2IB_β[p(z|x)] < 0$ at the trivial representation $p(z|x) = p(z)$.

The proof for Theorem 3 is given in Appendix D. Intuitively, if $δ^2IB_β[p(z|x)]|_{p(z|x)=p(z)} < 0$, we can always find a $p'(z|x) = p(z|x) + ϵ · h(z|x)$ in the neighborhood of the trivial representation $p(z|x) = p(z)$, such that $IB_β[p'(z|x)] < IB_β[p(z|x)]$, thus satisfying the definition for $IB_β$-Learnability.

To make Theorem 3 more practical, we perturb $p(z|x)$ around the trivial solution $p'(z|x) = p(z|x) + ϵ · h(z|x)$, and expand $IB_β[p(z|x) + ϵ · h(z|x)] - IB_β[p(z|x)]$ to the second order of $ϵ$. We can then prove Theorem 4.

**Theorem 4 (Suff. Cond. 2).** A sufficient condition for $(X, Y)$ to be $IB_β$-learnable is $X$ and $Y$ are not independent, and

$$β > \inf_{h(x)} β_0[h(x)] \tag{2}$$

where the functional $β_0[h(x)]$ is given by

$$β_0[h(x)] = \frac{E_{x \sim p(x)}[h(x)^2] - (E_{x \sim p(x)}[h(x)])^2}{E_{y \sim p(y)}[E_{x \sim p(x|y)}[h(x)]^2] - (E_{x \sim p(x)}[h(x)])^2}$$

Moreover, we have that $\left(\inf_{h(x)} β[h(x)]\right)^{-1}$ is a lower bound of the slope of the Pareto frontier in the information plane $I(Y; Z)$ vs. $I(X; Z)$ at the origin.
The proof is given in Appendix C, which also shows that if \( \beta > \inf_{h(x)} \beta_0[h(x)] \) in Theorem 3 is satisfied, we can construct a perturbation function \( h(z|x) = h^*(x)h_2(z) \) with \( h^*(x) = \arg \min_{h(x)} \beta_0[h(x)] \), \( \int h_2(z)dz = 0 \), \( \int h^2_2(z)dz > 0 \) for some \( h_2(z) \), such that \( h(z|x) \) satisfies Theorem 3. It also shows that the converse is true: if there exists \( h(z|x) \) such that the condition in Theorem 3 is true, then Theorem 4 is satisfied, i.e., \( \beta > \inf_{h(x)} \beta_0[h(x)] \). Moreover, letting the perturbation function \( h(z|x) = h^*(x)h_2(z) \) at the trivial solution, we have

\[
p_{\beta}(y|x) = p(y) + e^{2C_\beta}(h^*(x) - \bar{h}_x) \cdot \int p(x,y)(h^*(x) - \bar{h}_x)dx \tag{3}
\]

where \( p_{\beta}(y|x) \) is the estimated \( p(y|x) \) by IB for a certain \( \beta, \bar{h}_x = \int h^*(x)p(x)dx \), and \( C_\beta = \int h^2_2(z)p(z)dz > 0 \) is a constant. This shows how the \( p_{\beta}(y|x) \) by IB explicitly depends on \( h^*(x) \) at the onset of learning. The proof is provided in Appendix 4.

Theorem 4 suggests a method to estimate \( \beta_0 \): we can parameterize \( h(x) \) e.g., by a neural network, with the objective of minimizing \( \beta_0[h(x)] \). At its minimization, \( \beta_0[h(x)] \) provides an upper bound for \( \beta_0 \), and \( h(x) \) provides a soft clustering of the examples corresponding to a nontrivial perturbation of \( p(z|x) \) at \( p(z|x) = p(z) \) that minimizes \( \text{IB}_\beta[p(z|x)] \).

Alternatively, based on the property of \( \beta_0[h(x)] \), we can also use a specific functional form for \( h(x) \) in Eq. (5), and obtain a stronger sufficient condition for \( \text{IB}_\beta \)-Learnability. But we want to choose \( h(x) \) as near to the infimum as possible. To do this, we note the following characteristics for the R.H.S of Eq. (4):

- We can set \( h(x) \) to be nonzero if \( x \in \Omega_x \) for some region \( \Omega_x \subset \mathcal{X} \) and 0 otherwise. Then we obtain the following sufficient condition:

\[
\beta > \inf_{h(x),\Omega_x \subset \mathcal{X}} \frac{\mathbb{E}_{y \sim p(y|x)} [h(x)^2]}{\mathbb{E}_{y \sim p(y|x)} [p(y|h(x))]} - 1 \cdot \int \frac{dy}{p(y)} \left( \frac{\mathbb{E}_{y \sim p(y|x)} [p(y|h(x))]}{\mathbb{E}_{y \sim p(y|x)} [p(y|h(x))]} - 1 \right)^2 dx \tag{4}
\]

- The numerator of the R.H.S. of Eq. (4) attains its minimum when \( h(x) \) is a constant within \( \Omega_x \).

This can be proved using the Cauchy-Schwarz inequality: \( \langle u, v \rangle \geq \langle u, u \rangle \), setting \( u(x) = h(x)\sqrt{p(x)}, v(x) = \sqrt{p(x)} \), and defining the inner product as \( \langle u, v \rangle = \int u(x)v(x)dx \). Therefore, the numerator of the R.H.S. of Eq. (4) \( \geq \frac{1}{\int_{x \in \Omega_x} p(x) - 1} \), and attains equality when \( \frac{u(x)}{v(x)} = h(x) \) is constant.

Based on these observations, we can let \( h(x) \) be a nonzero constant inside some region \( \Omega_x \subset \mathcal{X} \) and otherwise, and the infimum over an arbitrary function \( h(x) \) is simplified to infimum over \( \Omega_x \subset \mathcal{X} \), and we obtain a sufficient condition for \( \text{IB}_\beta \)-Learnability, which is a key result of this paper:

**Theorem 5 (Conspicuous Subset Suff. Cond.).** A sufficient condition for \((X, Y)\) to be \( \text{IB}_\beta \)-learnable is \( X \) and \( Y \) are not independent, and

\[
\beta > \inf_{\Omega_x \subset \mathcal{X}} \beta_0(\Omega_x) \tag{5}
\]

where

\[
\beta_0(\Omega_x) = \frac{1}{\mathbb{E}_{y \sim p(y|\Omega_x)} [p(y|\Omega_x)]} - 1
\]

\( \Omega_x \) denotes the event that \( x \in \Omega_x \), with probability \( p(\Omega_x) \).

\( \beta_0(\Omega_x) \) gives a lower bound of the slope of the Pareto frontier in the information plane \( I(Y; Z) \) vs. \( I(X; Z) \) at the origin.

The proof is given in Appendix D. In the proof we also show that this condition is invariant to invertible mappings of \( X \).

5 Discussion

The conspicuous subset determines \( \beta_0 \). From Eq. (5), we see that three characteristics of the subset \( \Omega_x \subset \mathcal{X} \) lead to low \( \beta_0 \): (1) confidence: \( p(y|\Omega_x) \) is large; (2) typicality and size: the number of elements in \( \Omega_x \) is large, or the elements in \( \Omega_x \) are typical, leading to a large probability of \( p(\Omega_x) \); (3) imbalance: \( p(y) \) is small for the subset \( \Omega_x \), but large for its complement. In summary, \( \beta_0 \) will be determined by the largest confident, typical and imbalanced subset of examples, or an equilibrium of those characteristics. We term \( \Omega_x \) at the minimization of \( \beta_0(\Omega_x) \) the conspicuous subset.

Multiple phase transitions. Based on this characterization of \( \Omega_x \), we can hypothesize datasets with multiple learnability phase transitions. Specifically, consider a region \( \Omega_{x0} \) that is small but "typical", consists of all elements confidently predicted as \( y_{00} \) by \( p(y|x) \), and where


\[ I(Y;Z) \text{[bits]} \]

0.1 0.2

\[ \Omega \]

\[ \sim \]

\[ \rho \]

\[ \log \]

\[ \frac{1}{p(\Omega_x)} - 1 \geq \log \frac{1}{p(\Omega_x)} = -\log p(\Omega_x) = h(\Omega_x) \]

so we can estimate the phase transition as:

\[ \beta \gtrapprox \inf_{\Omega_x \subset \mathcal{X}} \frac{h(\Omega_x)}{I(\Omega_x; Y)} \tag{6} \]

Since Eq. (6) uses upper bounds on both the numerator and the denominator, it does not give us a bound on \( \beta_0 \).

\textbf{Estimating model capacity.} The observation that a model can’t distinguish between cluster overlap in the data and its own lack of capacity gives an interesting way to use IB-Learnability to measure the capacity of a set of models relative to the task they are being used to solve.

\textbf{Learnability and the Information Plane.} Many of our results can be interpreted in terms of the geometry of the Pareto frontier illustrated in Fig. 2 which describes the trade-off between increasing \( I(Y; Z) \) and decreasing \( I(X; Z) \). At any point on this frontier that minimizes \( \text{IB}_{Y} \equiv \min I(X; Z) - \beta I(Y; Z) \), the frontier will have slope \( \beta^{-1} \) if it is differentiable. If the frontier is also concave (has negative second derivative), then this slope \( \beta^{-1} \) will take its maximum \( \beta_0^{-1} \) at the origin, which implies IB-\( \beta \)-Learnability for \( \beta > \beta_0 \), so that the threshold for IB-\( \beta \)-Learnability is simply the inverse slope of the frontier at the origin. More generally, as long as the Pareto frontier is differentiable, the threshold for IB-\( \beta \)-learnability is the inverse of its maximum slope. Indeed, Theorem 4 and Theorem 5 give lower bounds of the slope of the Pareto frontier at the origin.

\textbf{IB-Learnability, hypercontractivity, and maximum correlation.} IB-Learnability and its sufficient conditions we provide harbor a deep connection with hypercontractivity and maximum correlation:

\[ \frac{1}{\beta_0} = \xi(X; Y) = \eta_{KL} \geq \sup_{h(x)} \frac{1}{\beta_0 |h(x)|} = \rho_m^2(X; Y) \tag{7} \]

which we prove in Appendix K. Here \( \rho_m(X; Y) \equiv \max_{f,g} \mathbb{E}[f(X)f(Y)] \text{ s.t. } \mathbb{E}[f(X)] = \mathbb{E}[g(Y)] = 0 \) and \( \mathbb{E}[f^2(X)] = \mathbb{E}[g^2(Y)] = 1 \) is the maximum correlation \[ \text{Hirschfeld} \text{ [1935], Gebelein} \text{ [1941], } \xi(X; Y) \equiv \sup_{Z \sim X \sim Y} \frac{I(Y; Z)}{I(X; Z)} \text{ is the hypercontractivity coefficient,} \]
and $\eta_{KL}(p(y|x), p(x)) \equiv \sup_{r(x) \neq p(x)} \frac{D_{KL}(r(y)||p(y))}{\eta_{KL}(r(x)||p(x))}$ is the contraction coefficient. Our proof relies on Anan-tharam et al. (2013)’s proof $\xi(X; Y) = \eta_{KL}$. Our work reveals the deep relationship between IB-Learnability and these earlier concepts and provides additional insights about what aspects of a dataset give rise to high maximum correlation and hypercontractivity: the most confident, typical, imbalanced subset of $(X, Y)$.

6 ESTIMATING THE IB-LEARNABILITY CONDITION

Theorem 5 not only reveals the relationship between the learnability threshold for $\beta$ and the least noisy region of $P(Y|X)$, but also provides a way to practically estimate $\beta_0$, both in the general classification case, and in more structured settings.

6.1 Estimation Algorithm

Based on Theorem 5, for general classification tasks we suggest Algorithm 1 to empirically estimate an upper-bound $\tilde{\beta}_0 \geq \beta_0$, as well as discovering the conspicuous subset that determines $\beta_0$.

We approximate the probability of each example $p(x_i)$ by its empirical probability, $\hat{p}(x_i)$. E.g., for MNIST, $p(x_i) = \frac{1}{N}$, where $N$ is the number of examples in the dataset. The algorithm starts by first learning a maximum likelihood model of $p_0(y|x)$, using e.g. feed-forward neural networks. It then constructs a matrix $P_{y|x}$ and a vector $p_y$ to store the estimated $p(y|x)$ and $p(y)$ for all the examples in the dataset. To find the subset $\Omega$ such that the $\tilde{\beta}_0$ is as small as possible, by previous analysis we want to find a conspicuous subset such that its $p(y|x)$ is large for a certain class $j$ (to make the denominator of Eq. 3 large), and containing as many elements as possible (to make the numerator small).

We suggest the following heuristics to discover such a conspicuous subset. For each class $j$, we sort the rows of $(P_{y|x})$ according to its probability for the pivot class $j$ by decreasing order, and then perform a search over $i_{\text{left}}, i_{\text{right}}$ for $\Omega = \{i_{\text{left}}, i_{\text{left}} + 1, ..., i_{\text{right}}\}$. Since $\tilde{\beta}_0$ is large when $\Omega$ contains too few or too many elements, the minimum of $\tilde{\beta}_{0(j)}$ for class $j$ will typically be reached with some intermediate-sized subset, and we can use binary search or other discrete search algorithm for the optimization. The algorithm stops when $\tilde{\beta}_{0(j)}$ does not improve by tolerance $\varepsilon$. The algorithm then returns the $\tilde{\beta}_0$ as the minimum over all the classes $\tilde{\beta}_{0(1)}, ..., \tilde{\beta}_{0(N)}$, as well as the conspicuous subset that determines this $\tilde{\beta}_0$.

Algorithm 1 Estimating the upper bound for $\beta_0$ and identifying the conspicuous subset

**Require**: Dataset $\mathcal{D} = \{(x_i, y_i)\}, i = 1, 2, ..., N$. The number of classes is $C$.

**Require**: $\varepsilon$: tolerance for estimating $\beta_0$

1: Learn a maximum likelihood model $p_0(y|x)$ using the dataset $\mathcal{D}$.
2: Construct matrix $(P_{y|x})$ such that $(P_{y|x})_{ij} = p_0(y = j|x = x_i)$.
3: Construct vector $p_y = (p_{y1}, ..., p_{yC})$ such that $p_{yj} = \frac{1}{N} \sum_{i=1}^{N} (P_{y|x})_{ij}$.
4: for $j$ in $\{1, 2, ..., C\}$:
5: $P_{y|x}^{(j)}$ ← Sort the rows of $P_{y|x}$ in decreasing values of $(P_{y|x})_{ij}$.
6: $\tilde{\beta}_0^{(j)}, \Omega^{(j)}$ ← Search $i_{\text{left}}, i_{\text{right}}$ to $\tilde{\beta}_0^{(j)} = \text{Get}\beta(P_{y|x}, p_y, \Omega)$ is minimal with tolerance $\varepsilon$, where $\Omega = \{i_{\text{left}}, i_{\text{left}} + 1, ..., i_{\text{right}}\}$.
7: end for
8: $j^* \leftarrow \arg\min_j \{\tilde{\beta}_0^{(j)}\}, j = 1, 2, ..., N$.
9: $\tilde{\beta}_0 \leftarrow \tilde{\beta}_{0}^{(j^*)}$.
10: $P_{y|x}^{(\tilde{\beta}_0)}$ ← the rows of $P_{y|x}^{(\tilde{\beta}_0)}$ indexed by $\Omega^{(j^*)}$.
11: return $\tilde{\beta}_0, P_{y|x}^{(\tilde{\beta}_0)}$

**subroutine Getβ(P_{y|x}, p_y, Ω):**

s1: $N \leftarrow$ number of rows of $P_{y|x}$.

s2: $C \leftarrow$ number of columns of $P_{y|x}$.

s3: $n \leftarrow$ number of elements of $\Omega$.

s4: $(P_{y|\Omega})_{j} \leftarrow \frac{1}{n} \sum_{i \in \Omega} (P_{y|x})_{ij}, j = 1, 2, ..., C$.

s5: $\tilde{\beta}_0 \leftarrow \frac{\sum_{j} [(P_{y|\Omega})_{j}]^2 - 1}{\sum_{j} (P_{y|\Omega})_{j}^2}$.

s6: return $\tilde{\beta}_0$

IB, either directly, or as an anchor for a region where we can perform a much smaller sweep than we otherwise would have. This may be particularly important for very noisy datasets, where $\beta_0$ can be very large.

6.2 Special Cases for Estimating $\beta_0$

Theorem 5 may still be challenging to estimate, due to the difficulty of making accurate estimates of $p(\Omega_x)$ and searching over $\Omega_x \subset \mathcal{X}$. However, if the learning problem is more structured, we may be able to obtain a simpler formula for the sufficient condition.

**Class-conditional label noise.** Classification with noisy labels is a common practical scenario. An important noise model is that the labels are randomly flipped with some hidden class-conditional probabilities and we only observe the corrupted labels. This problem has been studied extensively (Angluin and Laird 1988; Natarajan...
et al., 2013; Liu and Tao, 2016; Xiao et al., 2015; Northcutt et al., 2017. If IB is applied to this scenario, how large \( \beta \) do we need? The following corollary provides a simple formula.

**Corollary 5.1.** Suppose that the true class labels are \( y^* \), and the input space belonging to each \( y^* \) has no overlap. We only observe the corrupted labels \( y \) with class-conditional noise \( p(y|x, y^*) = p(y|y^*) \), and \( Y \) is not independent of \( X \). We have that a sufficient condition for IB\( _\beta \)-Learnability is:

\[
\beta > \inf_{y^*} \frac{1}{\sum_{y} \frac{p(y|y^*)^2}{p(y)}} - 1
\]  

We see that under class-conditional noise, the sufficient condition reduces to a discrete formula which only depends on the noise rates \( p(y|y^*) \) and the true class probability \( p(y^*) \), which can be accurately estimated via e.g. Northcutt et al. (2017). Additionally, if we know that the noise is class-conditional, but the observed \( \beta_0 \) is greater than the R.H.S. of Eq. (8), we can deduce that there is overlap between the true classes. The proof of Corollary 5.1 is provided in Appendix J.

**Deterministic relationships.** Theorem 5 also reveals that \( \beta_0 \) relates closely to whether \( Y \) is a deterministic function of \( X \), as shown by Corollary 5.2.

**Corollary 5.2.** Assume that \( Y \) contains at least one value \( y \) such that its probability \( p(y) > 0 \). If \( Y \) is a deterministic function of \( X \) and not independent of \( X \), then a sufficient condition for IB\( _\beta \)-Learnability is \( \beta > 1 \).

The assumption in the corollary 5.2 is satisfied by classification, and certain regression problems. Combined with the necessary condition \( \beta > 1 \) for any dataset \((X, Y)\) to be IB\( _\beta \)-learnable (Section 5), we have that under the assumption, if \( Y \) is a deterministic function of \( X \), then a necessary and sufficient condition for IB\( _\beta \)-learnability is \( \beta > 1 \); i.e., its \( \beta_0 \) is 1. The proof of Corollary 5.2 is provided in Appendix J.

Therefore, in practice, if we find that \( \beta_0 > 1 \), we may infer that \( Y \) is not a deterministic function of \( X \). For a classification task, we may infer that either some classes have overlap, or the labels are noisy. However, recall that finite models may add effective class overlap if they have insufficient capacity for the learning task, as mentioned in Section 4. This may translate into a higher observed \( \beta_0 \), even when learning deterministic functions.

7 EXPERIMENTS

To test how the theoretical conditions for IB\( _\beta \)-learnability match with experiment, we apply them to synthetic data with varying noise rates and class overlap, MNIST binary classification with varying noise rates, and CIFAR10 classification, comparing with the \( \beta_0 \) found experimentally. We also compare with the algorithm in Kim et al. (2017) for estimating the hypercontractivity coefficient \((=1/\beta_0)\) via the contraction coefficient \( \eta_{KL} \). Experiment details are in Section L.

7.1 Synthetic Dataset Experiments

We construct a set of datasets from 2D mixtures of 2 Gaussians as \( X \) and the identity of the mixture component as \( Y \). We simulate two practical scenarios with these datasets: (1) noisy labels with class-conditional noise, and (2) class overlap. For (1), we vary the class-conditional noise rates. For (2), we vary class overlap by tuning the distance between the Gaussians. For each experiment, we sweep \( \beta \) with exponential steps, and observe \( I(X; Z) \) and \( I(Y; Z) \). We then compare the empirical \( \beta_0 \) indicated by the onset of above-zero \( I(X; Z) \) with predicted values for \( \beta_0 \).

**Classification with class-conditional noise.** In this experiment, we have a mixture of Gaussian distribution with 2 components, each of which is a 2D Gaussian with diagonal covariance matrix \( \Sigma = \text{diag}(0.25, 0.25) \). The two components have distance 16 (hence virtually no overlap) and equal mixture weight. For each \( x \), the label \( y \in \{0, 1\} \) is the identity of which component it belongs to. We create multiple datasets by randomly flipping the labels \( y \) with a certain noise rate \( \rho = P(y = 0|y^* = 1) = P(y = 1|y^* = 0) \). For each dataset, we train VIB models across a range of \( \beta \), and observe the onset

![Figure 3: Predicted vs. experimentally identified \( \beta_0 \).](image)
of learning via random $I(X; Z)$ (Observed). To test how different
perform in estimating $\beta_0$, we apply the following methods: (I) Corollary 5.1, since this is clas-
sification with class-conditional noise, and the two true
classes have virtually no overlap; (2) Alg. 1 true $p(y|x)$; (3) $\hat{\eta}_{KL}$
with true $p(y|x)$; (4) $\beta_0 | h(x)$] in
Eq. (2); (2’) Alg. 1 with $p(y|x)$ estimated by a neural net;
(3’) $\hat{\eta}_{KL}$ with the same $p(y|x)$ as in (2’). The results are
shown in Fig. 3 and in Appendix [L.1]

From Fig. 3 we see the following. (A) When using the true $p(y|x)$, both Alg. 1 and $\hat{\eta}_{KL}$
generally upper bound the empirical $\beta_0$, and Alg. 1 is generally tighter. (B) When
using the true $p(y|x)$, Alg. 1 and Corollary 5.1
give the same result. (C) Comparing Alg. 1 and $\hat{\eta}_{KL}$, both
of which use the same empirically estimated $p(y|x)$, both
approaches provide good estimation in the low-noise re-
gion; however, in the high-noise region, Alg. 1 gives
more precise values than $\hat{\eta}_{KL}$, indicating that Alg. 1 is
more robust to the estimation error of $p(y|x)$. (D) Eq. (2)
empirically upper bounds the experimentally observed
$\beta_0$, and gives almost the same result as theoretical esti-
mation in Corollary 5.1 and Alg. 1 with the true $p(y|x)$.

In the classification setting, this approach doesn’t require
any learned estimate of $p(y|x)$, as we can directly use the
empirical $p(y)$ and $p(x|y)$ from SGD mini-batches.

This experiment also shows that for dataset where the
signal-to-noise is small, $\beta_0$ can be very high. Instead of
blindly sweeping $\beta$, our result can provide guidance for
setting $\beta$ so learning can happen.

**Classification with class overlap.** In this experiment,
we test how different amounts of overlap among classes
influence $\beta_0$. We use the mixture of Gaussians with two
components, each of which is a 2D Gaussian with diag-
onal covariance matrix $\Sigma = \text{diag}(0.25, 0.25)$. The two
components have weights 0.6 and 0.4. We vary the
distance between the Gaussians from 8.0 down to 0.8 and
observe the $\beta_{0, \text{exp}}$. Since we don’t add noise to the
labels, if there were no overlap and a deterministic map
from $X$ to $Y$, we would have $\beta_0 = 1$ by Corollary 5.2.
The more overlap between the two classes, the more un-
certain $Y$ is given $X$. By Eq. 5 we expect $\beta_0$ to be larger,
which is corroborated in Fig. 4.

### 7.2 MNIST Experiments

We perform binary classification with digits 0 and 1, and
as before, add class-conditional noise to the labels with
varying noise rates $\rho$. To explore how the model capac-
ity influences the onset of learning, for each dataset we
train two sets of VIB models differing only by the num-
ber of neurons in their hidden layers of the encoder: one
with $n = 512$ neurons, the other with $n = 128$ neurons.

As we describe in Section 4, insufficient capacity will re-
sult in more uncertainty of $Y$ given $X$, so we expect the observed $\beta_0$ for the
$n = 128$ model to be larger. This result is confirmed by
Figure 6: Histograms of the full MNIST training and validation sets according to $h(X)$. Note that both are bimodal, and the histograms are indistinguishable. In both cases, $h(x)$ has learned to separate most of the ones into the smaller mode, but difficult ones are in the wide valley between the two modes. See Figure 8 for all of the training images to the left of the red threshold line, as well as the first few images to the right of the threshold.

7.3 MNIST Experiments using Equation 2

To see what IB learns at its onset of learning for the full MNIST dataset, we optimize Eq. (2) w.r.t. the full MNIST dataset, and visualize the clustering of digits by $h(x)$. Eq. (2) can be optimized using SGD using any differentiable parameterized mapping $h(x) : \mathcal{X} \rightarrow \mathbb{R}$. In this case, we chose to parameterize $h(x)$ with a PixelCNN++ architecture [Oord et al., 2016; Salimans et al., 2017], as PixelCNN++ is a powerful autoregressive model for images that gives a scalar output (normally interpreted as $\log p(x)$). Eq. (2) should generally give two clusters in the output space, as discussed in Section 4. In this setup, smaller values of $h(x)$ correspond to the subset of the data that is easiest to learn. Fig. 6 shows two strongly separated clusters, as well as the threshold we choose to divide them. Fig. 8 shows the first 5,776 MNIST training examples as sorted by our learned $h(x)$, with the examples above the threshold highlighted in red. We can clearly see that our learned $h(x)$ has separated the “easy” one (1) digits from the rest of the MNIST training set.

7.4 CIFAR10 Forgetting Experiments

For CIFAR10 [Krizhevsky and Hinton, 2009], we study how forgetting varies with $\beta$. In other words, given a VIB model trained at some high $\beta_2$, if we anneal it down to some much lower $\beta_1$, what $I(Y;Z)$ does the model converge to? Using Alg. 1 we estimated $\beta_0 = 1.0483$ on a version of CIFAR10 with 20% label noise, where the $P_{y|x}$ is estimated by maximum likelihood training with the same encoder and classifier architectures as used for VIB. For the VIB models, the lowest $\beta$ with performance above chance was $\beta = 1.048$, a very tight match with the estimate from Alg. 1. See Appendix L.2 for details.

8 CONCLUSION

In this paper, we have presented theoretical results for predicting the onset of learning, and have shown that it is determined by the conspicuous subset of the training examples. We gave a practical algorithm for predicting the transition as well as discovering this subset, and showed that those predictions are accurate, even in cases of extreme label noise. We believe these results will provide theoretical and practical guidance for choosing $\beta$ in the IB framework for balancing prediction and compression. Our work also raises other questions, such as whether there are other phase transitions in learnability that might be identified. We hope to address some of those questions in future work.

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Figure 8: The first 5776 MNIST training set digits when sorted by $h(x)$. The digits highlighted in red are above the threshold drawn in Figure 6.
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Appendix

The structure of the Appendix is as follows. In Section A, we provide preliminaries for the first-order and second-order variations on functionals. We prove Theorem 1 and Theorem 2 in Section B and C, respectively. In Section D, we prove the necessary condition for IB-learnability. In Section E, we prove the sufficient condition 1 for IB-learnability. In Section F, we calculate the first and second variations of IB_β[p(z|x)] at the trivial representation p(z|x) = p(z), which is used in proving the sufficient condition 2 for IB_β-learnability. In Section G, we prove Eq. (3) at the onset of learning. After these preparations, we prove the key result of this paper, Theorem 3, in Section H. Then two important corollaries are proved in Section I. In Section J, we explore the deep relation between β_α, β_β[h(x)], the hypercontractivity coefficient, contraction coefficient, and maximum correlation. Finally in Section K, we provide details for the experiments.

A Preliminaries: first-order and second-order variations

Let functional F[f(x)] be defined on some normed linear space R. Let us add a perturbative function ϵ · h(x) to f(x), and now the functional F[f(x) + ϵ · h(x)] can be expanded as

\[ \Delta F[f(x)] = F[f(x) + ϵ · h(x)] - F[f(x)] = \varphi_1[f(x)] + \varphi_2[f(x)] + O(ϵ^3)||h||^2 \]

where ||h|| denotes the norm of h. \( \varphi_1[f(x)] = \frac{dF[f(x)]}{dϵ} \) is a linear functional of ϵ · h(x), and is called the first-order variation, denoted as \( \delta F[f(x)] \). \( \varphi_2[f(x)] = \frac{1}{2} \cdot \delta^2 F[f(x)] \) is a quadratic functional of ϵ · h(x), and is called the second-order variation, denoted as \( \delta^2 F[f(x)] \).

If \( \delta F[f(x)] = 0 \), we call f(x) a stationary solution for the functional F[·]. If \( \Delta F[f(x)] \geq 0 \) for all h(x) such that f(x) + ϵ · h(x) is at the neighborhood of f(x), we call f(x) a (local) minimum of F[·].

B Proof of Theorem 1

Proof. If \( (X, Y) \) is IB_β-learnable, then there exists Z given by some \( p_1(z|x) \) such that IB_β(X, Y; Z) < IB(X, Y; Z_{trivial}) = 0, where Z_{trivial} satisfies p(z|x) = p(z). Since \( X' = g(X) \) is an invertible map (if X is continuous variable, \( g \) is additionally required to be continuous), and mutual information is invariant under such an invertible map (Kraskov et al. 2004), we have that IB_β(X', Y; Z) = I(X'; Z) - βI(Y; Z) = I(X; Z) - βI(Y; Z) = IB_β(X, Y; Z) < 0 = IB(X', Y; Z_{trivial}). So \( (X', Y) \) is IB_β-learnable. On the other hand, if \( (X, Y) \) is not IB_β-learnable, then \( \forall Z, \) we have IB_β(X, Y; Z) ≥ IB(X, Y; Z_{trivial}) = 0. Again using mutual information’s invariance under \( g \), we have for all Z, IB_β(X', Y; Z) = IB_β(X, Y; Z) ≥ IB(X, Y; Z_{trivial}) = 0, leading to that \( (X', Y) \) is not IB_β-learnable. Therefore, we have that \( (X, Y) \) and \( (X', Y) \) have the same IB_β-learnability.

C Proof of Theorem 2

Proof. At the trivial representation p(z|x) = p(z), we have I(X; Z) = 0, and I(Y; Z) = 0 due to the Markov chain, so IB_β(X, Y; Z)|_{p(z|x) = p(z)} = 0 for any β. Since \( (X, Y) \) is IB_β_1-learnable, there exists a Z given by a \( p_1(z|x) \) such that IB_β_1(X, Y; Z)|_{p_1(z|x) = p_1(z)} < 0. Since \( β_2 > β_1 \), and I(Y; Z) ≥ 0, we have IB_β_2(X, Y; Z)|_{p_1(z|x) = p_1(z)} ≤ IB_β_2(X, Y; Z)|_{p_1(z|x) = p_1(z)} < 0 = IB_β_2(X, Y; Z)|_{p(z|x) = p(z)}. Therefore, \( (X, Y) \) is IB_β_2-learnable.

D Proof of Theorem 3

Proof. To prove Theorem 3 we use the Theorem 1 of Chapter 5 of Gelfand et al. (2000) which gives a necessary condition for F[f(x)] to have a minimum at \( f_0(x) \). Adapting to our notation, we have:
Applying to our functional $IB_\beta[p(z|x)]$, an immediate result of Theorem 6, is that, if at $p(z|x) = p(z)$, there exists an $\epsilon \cdot h(z|x)$ such that $\delta^2 IB_\beta[p(z|x)] < 0$, then $p(z|x) = p(z)$ is not a minimum for $IB_\beta[p(z|x)]$. Using the definition of $IB_\beta$ learnability, we have that $(X, Y)$ is $IB_\beta$-learnable.

\[ \checkmark \]

E  First- and second-order variations of $IB_\beta[p(z|x)]$

In this section, we derive the first- and second-order variations of $IB_\beta[p(z|x)]$, which are needed for proving Lemma 2.1 and Theorem 4.

Lemma 6.1. Using perturbative function $h(z|x)$, we have

\begin{align*}
\delta IB_\beta[p(z|x)] &= \int dxdzp(x)h(z|x)\log \frac{p(z|x)}{p(z)} - \beta \int dxdydzp(x, y)h(z|x)\log \frac{p(z|y)}{p(z)} \\
\delta^2 IB_\beta[p(z|x)] &= \frac{1}{2} \left[ \int dxdz \frac{p(x)^2}{p(x, z)} h(z|x)^2 - \beta \int dxdx'dydz \frac{p(x, y)p(x', y)}{p(y, z)} h(z|x)h(z|x') + (\beta - 1) \int dxdx'dz \frac{p(x)p(x')}{p(z)} h(z|x)h(z|x') \right]
\end{align*}

Proof. Since $IB_\beta[p(z|x)] = I(X; Z) - \beta I(Y; Z)$, let us calculate the first and second-order variation of $I(X; Z)$ and $I(Y; Z)$ w.r.t. $p(z|x)$, respectively. Through this derivation, we use $\epsilon h(z|x)$ as a perturbative function, for ease of deciding different orders of variations. We will finally absorb $\epsilon$ into $h(z|x)$.

Denote $I(X; Z) = F_1[p(z|x)]$. We have

\[ F_1[p(z|x)] = I(X; Z) = \int dxdzp(z|x)p(x)\log \frac{p(z|x)}{p(z)} \]

Since

\[ p(z) = \int p(z|x)p(x)dx \]

We have

\[ p(z)|_{p(z|x)+\epsilon h(z|x)} = p(z)|_{p(z|x)} + \epsilon \int h(z|x)p(x)dx \]

Expanding $F_1[p(z|x) + \epsilon h(z|x)]$ to the second order of $\epsilon$, we have
$F_1[p(z|x) + \epsilon h(z|x)]$

\[
\begin{align*}
&= \int dx dz p(x)p(z|x + \epsilon h(z|x))\log \frac{p(z|x) + \epsilon h(z|x)}{p(z)} + \epsilon \int h(z|x)p(x'|z|x)dx' \\
&= \int dx dz p(x)p(z|x) \left(1 + \epsilon \frac{h(z|x)}{p(z|x)}\right) \log \frac{p(z|x)}{p(z)} \left(1 + \epsilon \frac{h(z|x)}{p(z|x)}\right) \left(1 - \epsilon \int h(z|x)p(x'|z|x)dx'\right) \\
&\quad + \epsilon^2 \left( \frac{\int h(z|x)p(x'|z|x)dx'}{p(z)} \right)^2 + O(\epsilon^3) \\
&= \int dx dz p(x)p(z|x) \left(1 + \epsilon \frac{h(z|x)}{p(z|x)}\right) \log \left[\frac{p(z|x)}{p(z)} \left(1 + \epsilon \frac{h(z|x)}{p(z|x)}\right) \left(1 - \epsilon \int h(z|x)p(x'|z|x)dx'\right)\right] \\
&\quad + \epsilon^2 \left( \frac{\int h(z|x)p(x'|z|x)dx'}{p(z)} \right)^2 - \epsilon^2 \frac{h(z|x)}{p(z|x)} \int h(z|x)p(x'|z|x)dx' + O(\epsilon^3) \\
&= \int dx dz p(x)p(z|x) h(z|x) - \epsilon \int dx dz p(x)p(z|x) h(z|x) + \epsilon \int dx dz p(x)p(z|x) \log \frac{p(z|x)}{p(z)} \\
&\quad + \epsilon^2 \left( \frac{\int h(z|x)p(x'|z|x)dx'}{p(z)} \right)^2 - \epsilon^2 \frac{h(z|x)}{p(z|x)} \int h(z|x)p(x'|z|x)dx' - \frac{1}{2} \epsilon^2 \left( \frac{h(z|x)}{p(z|x)} - \frac{\int h(z|x)p(x'|z|x)dx'}{p(z)} \right)^2 + O(\epsilon^3)
\end{align*}
\]

Collecting the first order terms of $\epsilon$, we have

\[
\delta F_1[p(z|x)] = \epsilon \int dx dz p(x)p(z|x) h(z|x) + \epsilon \int dx dz p(x)p(z|x) \log \frac{p(z|x)}{p(z)}
\]

Collecting the second order terms of $\epsilon^2$, we have

\[
\delta^2 F_1[p(z|x)] = \epsilon^2 \int dx dz p(x)p(z|x) \left( \frac{\int h(z|x)p(x'|z|x)dx'}{p(z)} \right)^2 - \epsilon^2 \frac{h(z|x)}{p(z|x)} \int h(z|x)p(x'|z|x)dx' - \frac{1}{2} \epsilon^2 \left( \frac{h(z|x)}{p(z|x)} - \frac{\int h(z|x)p(x'|z|x)dx'}{p(z)} \right)^2
\]

Now let us calculate the first and second-order variation of $F_2[p(z|x)] = I(Z; Y)$. We have

\[
F_2[p(z|x)] = I(Y; Z) = \int dy dz p(z|y)p(y) \log \frac{p(y,z)}{p(y)p(z)} = \int dx dy dz p(z|y)p(x|y) \log \frac{p(y,z)}{p(y)p(z)}
\]

Using the Markov chain $Z \sim X \sim Y$, we have

\[
p(y,z) = \int p(z|x)p(x,y)dx
\]
Hence
\[ p(y, z)|_{p(z|x)} + \epsilon h(z|x) = p(y, z)|_{p(z|x)} + \epsilon \int h(z|x)p(x, y)dx \]

Then expanding \( F_2[p(z|x) + \epsilon h(z|x)] \) to the second order of \( \epsilon \), we have

\[
F_2[p(z|x) + \epsilon h(z|x)]
\]
\[ = \int dx dy dz p(x, y)p(z|x) \left( 1 + \frac{h(z|x)}{p(z|x)} \right) \log p(y, z) \left( 1 + \frac{\int h(z|x')p(x', y)dx'}{p(y)p(z)} \right) + \epsilon \left( \int dx dy dz p(x, y)p(z|x) \left( \frac{h(z|x')p(x', y)dx'}{p(z)} \right) - \frac{1}{2} \left( \frac{\int h(z|x')p(x', y)dx'}{p(y)p(z)} \right)^2 \right)
\]

Collecting the first order terms of \( \epsilon \), we have

\[
\delta F_2[p(z|x)]
\]
\[ = \epsilon \int dx dy dz p(x, y)h(z|x)\log \frac{p(y, z)}{p(y)p(z)} + \epsilon \int dx dy dz p(x, y)p(z|x) \int h(z|x')p(x', y)dx' \]
\[ - \epsilon \int dx dy dz p(x, y)p(z|x) \int h(z|x')p(x', y)dx' \]
\[ = \epsilon \int dx dy dz p(x, y)h(z|x)\log \frac{p(y, z)}{p(y)p(z)} + \epsilon \int dx' dy dz h(z|x')p(x', y) - \epsilon \int dz h(z|x')p(x')dx' \]

Collecting the second order terms of \( \epsilon \), we have

\[
\delta^2 F_2[p(z|x)]
\]
\[ = \epsilon^2 \int dx dy dz p(x, y)p(z|x) \left( \left( \frac{\int h(z|x')p(x', y)dx'}{p(z)} \right)^2 - \frac{\int h(z|x')p(x', y)dx' \int h(z|x'')p(x'', y)dx''}{p(z)} \right)
\]
\[ - \frac{\epsilon^2}{2} \int dx dy dz p(x, y)p(z|x) \left( \frac{\int h(z|x')p(x', y)dx'}{p(z)} \right)^2 - \frac{\int h(z|x')p(x', y)dx' \int h(z|x'')p(x'', y)dx''}{p(z)} \right)
\]
\[ + \epsilon^2 \int dx dy dz p(x, y)p(z|x) \left( \frac{h(z|x)}{p(y)p(z)} \right) \left( \frac{\int h(z|x')p(x', y)dx'}{p(y)p(z)} \right) - \frac{\int h(z|x')p(x', y)dx' \int h(z|x'')p(x'', y)dx''}{p(z)} \right)
\]
\[ = \frac{\epsilon^2}{2} \int dx dy dz \frac{p(x, y)p(z|x)}{p(y)p(z)} h(z|x)h(z|x') - \frac{\epsilon^2}{2} \int dx dy dz \frac{p(x|z)p(z|x)}{p(z)} h(z|x)h(z|x') \]

Finally, we have

\[
\delta IB_{p|z} = \delta F_1[p(z|x)] - \beta \cdot \delta F_2[p(z|x)]
\]
\[ = \epsilon \left( \int dx dy dz p(x, y)h(z|x)\log \frac{p(z|x)}{p(z)} - \beta \int dx dy dz p(x, y)h(z|x)\log \frac{p(z|x)}{p(z)} \right)
\]
\[ \delta^2 \text{IB}_\beta[p(z|x)] = \delta^2 F_1[p(z|x)] - \beta \cdot \delta^2 F_2[p(z|x)] \]

\[
= \frac{\epsilon^2}{2} \int dx dz \frac{B(x)^2}{p(x, z)} h(z|x)^2 - \frac{\epsilon^2}{2} \int dx dx' dz \frac{p(x)p(x')}{p(z)} h(z|x) h(z|x') \\
- \beta \epsilon^2 \left[ \frac{1}{2} \int dx dx' dy dz \frac{p(x, y)p(x', y)}{p(y) p(z)} h(z|x) h(z|x') - \frac{1}{2} \int dx dx' dz \frac{p(x)p(x')}{p(z)} h(z|x) h(z|x') \right] \\
= \frac{\epsilon^2}{2} \left[ \int dx dz \frac{p(x)^2}{p(x, z)} h(z|x)^2 \\
- \beta \int dx dx' dy dz \frac{p(x, y)p(x', y)}{p(y) p(z)} h(z|x) h(z|x') + (\beta - 1) \int dx dx' dz \frac{p(x)p(x')}{p(z)} h(z|x) h(z|x') \right]
\]

Absorb \( \epsilon \) into \( h(z|x) \), we get rid of the \( \epsilon \) factor and obtain the final expression in Lemma 6.1.

\[ \square \]

\section*{F Proof of Lemma 2.1}

\textit{Proof.} Using Lemma 6.1 we have

\[ \delta \text{IB}_\beta[p(z|x)] = \int dx dz p(x) h(z|x) \log \frac{p(z|x)}{p(z)} = \beta \int dx dy dz p(x, y) h(z|x) \log \frac{p(z|y)}{p(z)} \]

Let \( p(z|x) = p(z) \) (the trivial representation), we have that \( \log \frac{p(z|x)}{p(z)} \equiv 0 \). Therefore, the two integrals are both 0. Hence,

\[ \delta \text{IB}_\beta[p(z|x)] \big|_{p(z|x)=p(z)} \equiv 0 \]

Therefore, the \( p(z|x) = p(z) \) is a stationary solution for \( \text{IB}_\beta[p(z|x)] \).

\[ \square \]

\section*{G Proof of Theorem 4}

\textit{Proof.} Firstly, from the necessary condition of \( \beta > 1 \) in Section 3 we have that any sufficient condition for \( \text{IB}_\beta \)-learnability should be able to deduce \( \beta > 1 \).

Now using Theorem 3, a sufficient condition for \( (X, Y) \) to be \( \text{IB}_\beta \)-learnable is that there exists \( h(z|x) \) with \( \int h(z|x) dx = 0 \) such that \( \delta^2 \text{IB}_\beta[p(z|x)] < 0 \) at \( p(z|x) = p(x) \).

At the trivial representation, \( p(z|x) = p(z) \) and hence \( p(x, z) = p(x) p(z) \). Due to the Markov chain \( Z \leftarrow X \leftrightarrow Y \), we have \( p(y, z) = p(y)p(z) \). Substituting them into the \( \delta^2 \text{IB}_\beta[p(z|x)] \) in Lemma 6.1, the condition becomes: there exists \( h(z|x) \) with \( \int h(z|x) dz = 0 \), such that

\[
0 > \delta^2 \text{IB}_\beta[p(z|x)] = \\
\frac{1}{2} \left[ \int dx dz \frac{p(x)^2}{p(x)p(z)} h(z|x)^2 - \beta \int dx dx' dy dz \frac{p(x, y)p(x', y)}{p(y) p(z)} h(z|x) h(z|x') + (\beta - 1) \int dx dx' dz \frac{p(x)p(x')}{p(z)} h(z|x) h(z|x') \right] \\
(10)
\]

Rearranging terms and simplifying, we have

\[
\int \frac{dz}{p(z)} G[h(z|x)] = \int \frac{dz}{p(z)} \left[ \int dx h(z|x)^2 p(x) - \beta \int \frac{dy}{p(y)} \left( \int dx h(z|x)p(x|y) \right)^2 + (\beta - 1) \left( \int dx h(z|x)p(x) \right)^2 \right] < 0
\]

where

\[ G[h(x)] = \int dx h(x)^2 p(x) - \beta \int \frac{dy}{p(y)} \left( \int dx h(x)p(x|y) \right)^2 + (\beta - 1) \left( \int dx h(x)p(x) \right)^2 \]
Now we prove that the condition that \( \exists h(z|x) \) s.t. \( \int \frac{dz}{p(z)} G(h(z|x)) < 0 \) is equivalent to the condition that \( \exists h(x) \) s.t. \( G(h(x)) < 0 \).

If \( \forall h(z|x), G(h(z|x)) \geq 0 \), then we have \( \forall h(z|x), \int \frac{dz}{p(z)} G(h(z|x)) \geq 0 \). Therefore, if \( \exists h(z|x) \) s.t. \( \int \frac{dz}{p(z)} G(h(z|x)) < 0 \), we have that \( \exists h(z|x) \) s.t. \( G(h(z|x)) < 0 \). Since the functional \( G(h(z|x)) \) does not contain integration over \( z \), we can treat the \( z \) in \( G(h(z|x)) \) as a parameter and we have that \( \exists h(x) \) s.t. \( G(h(x)) < 0 \).

Conversely, if there exists an certain function \( h(x) \) such that \( G(h(x)) < 0 \), we can find some \( h_2(z) \) such that \( \int h_2(z)dz = 0 \) and \( \int \frac{h_2^2(z)}{p(z)} dz > 0 \), and let \( h_1(z|x) = h(x)h_2(z) \). Now we have

\[
\int \frac{dz}{p(z)} G(h(z|x)) = \int \frac{h_2^2(z)dz}{p(z)} G(h(x)) = G(h(x)) \int \frac{h_2^2(z)dz}{p(z)} < 0
\]

In other words, the condition Eq. (10) is equivalent to requiring that there exists an \( h(x) \) such that \( G(h(x)) < 0 \).

Hence, a sufficient condition for IB\(_\beta\)-learnability is that there exists an \( h(x) \) such that

\[
G(h(x)) = \int dxh(x)^2p(x) - \beta \int \frac{dy}{p(y)} \left( \int dxh(x)p(x)p(y|x) \right)^2 + (\beta - 1) \left( \int dxh(x)p(x) \right)^2 < 0 \tag{11}
\]

When \( h(x) = C = \text{constant} \) in the entire input space \( \mathcal{X} \), Eq. (11) becomes:

\[
C^2 - \beta C^2 + (\beta - 1)C^2 < 0
\]

which cannot be true. Therefore, \( h(x) = \text{constant} \) cannot satisfy Eq. (11).

Rearranging terms and simplifying, and note that \( \left( \int dxh(x)p(x) \right)^2 > 0 \) due to \( h(x) \neq 0 \) = constant, we have

\[
\beta \left[ \int \frac{dy}{p(y)} \left( \int dxh(x)p(x)p(y|x) \right)^2 \right] - 1 > \frac{\int dxh(x)^2p(x)}{\left( \int dxh(x)p(x) \right)^2} - 1 \tag{12}
\]

For the R.H.S. of Eq. (12), let us show that it is greater than 0. Using Cauchy-Schwarz inequality: \( \langle u, u \rangle (v, v) \geq \langle u, v \rangle^2 \), and setting \( u(x) = h(x)\sqrt{p(x)} \), \( v(x) = \sqrt{p(x)} \), and defining the inner product as \( \langle u, v \rangle = \int u(x)v(x)dx \). We have

\[
\frac{\int dxh(x)^2p(x)}{\left( \int dxh(x)p(x) \right)^2} \geq \frac{1}{p(x)dx} = 1
\]

It attains equality when \( \frac{u(x)}{v(x)} = h(x) \) is constant. Since \( h(x) \) cannot be constant, we have that the R.H.S. of Eq. (12) is greater than 0.

For the L.H.S. of Eq. (12), due to the necessary condition that \( \beta > 0 \), \[ \left[ \frac{\int \frac{dy}{p(y)} \left( \int dxh(x)p(x)p(y|x) \right)^2}{\left( \int dxh(x)p(x) \right)^2} - 1 \right] \leq 0 \], Eq. (12) cannot hold. Then the \( h(x) \) such that Eq. (12) holds is for those that satisfies

\[
\int \frac{dy}{p(y)} \left( \int dxh(x)p(x)p(y|x) \right)^2 \left( \int dxh(x)p(x) \right)^2 - 1 > 0
\]

i.e.

\[
\int dy p(y) \left( \int dxp(x|h(x)) \right)^2 > \left( \int dxp(x)h(x) \right)^2
\]

We see this constraint contains the requirement that \( h(x) \neq \text{constant} \).
Written in the form of expectations, we have

\[ \mathbb{E}_{y \sim p(y)} \left( \mathbb{E}_{x \sim p(x|y)} [h(x)] \right)^2 > \left( \mathbb{E}_{x \sim p(x)} [h(x)] \right)^2 \]  \hspace{1cm} (13)

Since the square function is convex, using Jensen’s inequality on the outer expectation on the L.H.S. of Eq. (13), we have

\[ \mathbb{E}_{y \sim p(y)} \left( \mathbb{E}_{x \sim p(x|y)} [h(x)] \right)^2 \geq \left( \mathbb{E}_{y \sim p(y)} [\mathbb{E}_{x \sim p(x|y)} [h(x)]] \right)^2 = \left( \mathbb{E}_{x \sim p(x)} [h(x)] \right)^2 \]

The equality holds iff \( \mathbb{E}_{x \sim p(x|y)} [h(x)] \) is constant w.r.t. \( y \), i.e. \( Y \) is independent of \( X \). Therefore, in order for Eq. (13) to hold, we require that \( Y \) is not independent of \( X \).

Using Jensen’s inequality on the inner expectation on the L.H.S. of Eq. (13), we have

\[ \mathbb{E}_{y \sim p(y)} \left( \mathbb{E}_{x \sim p(x|y)} [h(x)] \right)^2 \leq \mathbb{E}_{y \sim p(y)} [\mathbb{E}_{x \sim p(x|y)} [h(x)^2]] = \mathbb{E}_{x \sim p(x)} [h(x)^2] \]

(14)

The equality holds when \( h(x) \) is a constant. Since we require that \( h(x) \) is not a constant, we have that the equality cannot be reached.

Under the constraint that \( Y \) is not independent of \( X \), we can divide both sides of Eq. (11) and obtain the condition: there exists an \( h(x) \) such that

\[ \beta > \frac{\int dx h(x)^2 p(x)}{\left( \int dx h(x) p(x) \right)^2} - 1 \]

\[ \frac{\int dx h(x) p(x)}{\left( \int dx h(x) p(x) \right)^2} - 1 \]

i.e.

\[ \beta > \inf_{h(x)} \frac{\int dx h(x)^2 p(x)}{\left( \int dx h(x) p(x) \right)^2} - 1 \]

\[ \frac{\int dx h(x) p(x)}{\left( \int dx h(x) p(x) \right)^2} - 1 \]

Written in the form of expectations, we have

\[ \beta > \inf_{h(x)} \mathbb{E}_{x \sim p(x)} [h(x)^2] \frac{\mathbb{E}_{x \sim p(x)} [h(x)]}{\left( \mathbb{E}_{x \sim p(x)} [h(x)] \right)^2} - 1 \]

\[ \frac{\mathbb{E}_{x \sim p(x)} [h(x)^2]}{\left( \mathbb{E}_{x \sim p(x)} [h(x)] \right)^2} - 1 \]

\[ \frac{\mathbb{E}_{x \sim p(x)} [h(x)]}{\left( \mathbb{E}_{x \sim p(x)} [h(x)] \right)^2} - 1 \]

\[ \frac{\mathbb{E}_{x \sim p(x)} [h(x)^2]}{\left( \mathbb{E}_{x \sim p(x)} [h(x)] \right)^2} - 1 \]

We can absorb the constraint Eq. (13) into the above formula, and get

\[ \beta > \inf_{h(x)} \beta_0 [h(x)] \]
Therefore, we have
\[ \beta_0[h(x)] = \frac{\mathbb{E}_{x \sim p(x)}[h(x)^2]}{(\mathbb{E}_{x \sim p(x)}[h(x)])^2} - 1 \]

which proves the condition of Theorem 4.
Furthermore, from Eq. (14) we have
\[ \beta_0[h(x)] > 1 \]

for \( h(x) \neq \text{const} \), which satisfies the necessary condition of \( \beta > 1 \) in Section 3.

Proof of lower bound of slope of the Pareto frontier at the origin:
Now we prove the second statement of Theorem 4. Since \( \delta I(X; Z) = 0 \) and \( \delta I(Y; Z) = 0 \) according to Lemma 2.1, we have \( (\Delta I(Y; Z)/\Delta I(X; Z))^{-1} = (\delta^2 I(Y; Z)/\delta^2 I(X; Z))^{-1} \). Substituting into the expression of \( \delta^2 I(Y; Z) \) and \( \delta^2 I(X; Z) \) from Lemma 6.1, we have
\[
\begin{align*}
(\Delta I(Y; Z)/\Delta I(X; Z))^{-1} &= (\delta^2 I(Y; Z)/\delta^2 I(X; Z))^{-1} \\
&= \frac{\mathbb{E}_{x \sim p(x)}[h(x)^2]}{(\mathbb{E}_{x \sim p(x)}[h(x)])^2} - \frac{\mathbb{E}_{y \sim p(y)}[\mathbb{E}_{x \sim p(x)}[h(x)^2]]}{\mathbb{E}_{y \sim p(y)}[\mathbb{E}_{x \sim p(x)}[h(x)]]^2}
\end{align*}
\]

Therefore, \( (\inf_{h(z)} \beta_0[h(x)])^{-1} \) gives the largest slope of \( \Delta I(Y; Z) \) vs. \( \Delta I(X; Z) \) for perturbation function of the form \( h_2(z|x) = h(x)h_2(z) \) satisfying \( \int h_2(z)dz = 0 \) and \( \int h_2^2(z)dz > 0 \), which is a lower bound of slope of \( \Delta I(Y; Z) \) vs. \( \Delta I(X; Z) \) for all possible perturbation function \( h_1(z|x) \). The latter is the slope of the Pareto frontier of the \( I(Y; Z) \) vs. \( I(X; Z) \) curve at the origin.

Inflection point for general \( Z \): If we do not assume that \( Z \) is at the origin of the information plane, but at some general stationary solution \( Z^* \) with \( p(z|x) \), we define
\[ \beta^{(2)}[h(x)] = \left( \frac{\delta^{2}I(Y;Z)}{\delta^{2}I(X;Z)} \right)^{-1} = \frac{\frac{\partial^2}{\partial x^2} \int dx dz \frac{p(x)^2}{p_z(x)} h(z|x)^2 - \frac{\partial^2}{\partial x^2} \int dx dz' \frac{h(z|x)h(z|x')}{p(z)} h(z|x)h(z|x')}{\frac{\partial^2}{\partial x^2} \int dx dz \frac{p(x)^2}{p_z(x)} h(z|x)^2} \]

\[ = \frac{\int dx dz \frac{p(x)^2}{p_z(x)} h(z|x)^2 - \int dx dz' \frac{h(z|x)h(z|x')}{p(z)} h(z|x)h(z|x')}{\int dx dz \frac{p(x)^2}{p_z(x)} h(z|x)^2 - \int dx dz' \frac{h(z|x)h(z|x')}{p(z)} h(z|x)h(z|x')} \]

\[ = \int \frac{dz}{p(z)} \left[ \int \frac{dy}{p(y|z)} \left( \int dx \frac{p(x,y)}{p(x|z)} h(z|x)^2 - (\int dx p(x|h(z|x)))^2 \right) \right] \]

\[ = \int \frac{dz}{p(z)} \left[ \int \frac{dy}{p(y|z)} (\int dx p(x,y)h(z|x)^2)^2 - \frac{1}{p(z)} (\int dx p(x|h(z|x))^2 \right] \]

\[ = \int \frac{dz}{p(z)} \left[ \int \frac{dy}{p(y|z)} (\int dx p(x,y)h(z|x)^2)^2 - \frac{1}{p(z)} (\int dx p(x|h(z|x))^2 \right] \]

which reduces to \( \beta_0[h(x)] \) when \( p(z|x) = p(z) \). When

\[ \beta > \inf_{h(z|x)} \beta^{(2)}[h(z|x)] \]

it becomes a non-stable solution (non-minimum), and we will have other \( Z \) that achieves a better \( IB_\beta(X,Y;Z) \) than the current \( Z^* \).

**H What IB first learns at its onset of learning**

In this section, we prove that at the onset of learning, if letting \( h(z|x) = h^*(x)h_2(z) \), we have

\[ p_\beta(y|x) = p(y) + \epsilon^{2}C_z(h^*(x) - \bar{h}^*_z) \int p(x,y)(h^*(x) - \bar{h}^*_z)dx \]

where \( p_\beta(y|x) \) is the estimated \( p(y|x) \) by IB for a certain \( \beta \), \( h^*(x) = \inf_{h(x)} \beta_0[h(x)] \), \( \bar{h}^*_z = \int h^*(x)p(x)dx \), \( C_z = \int \frac{h^*_z(z)}{p(z)} dz \) is a constant.

**Proof.** In IB, we use \( p_\beta(z|x) \) to obtain \( Z \) from \( X \), then obtain the prediction of \( Y \) from \( Z \) using \( p_\beta(y|z) \). Here we use subscript \( \beta \) to denote the probability (density) at the optimum of IB_{\beta}[p(z|x)] at a specific \( \beta \). We have

\[ p_\beta(y|x) = \int p_\beta(y|z)p_\beta(z|x)dz \]

\[ = \int dz \frac{p_\beta(y,z)p_\beta(z|x)}{p_\beta(z)} \]

\[ = \int dz \frac{p_\beta(z|x)}{p_\beta(z)} \int p(x',y)p_\beta(z|x')dx' \]
When we have a small perturbation $\epsilon \cdot h(z|x)$ at the trivial representation, $p_\beta(z|x) = p_\beta_0(z) + \epsilon \cdot h(z|x)$, we have $p_\beta(z) = p_\beta_0(z) + \epsilon \cdot \int h(z|x')p(x')dx'$. Substituting, we have

$$p_\beta(y|x) = \int dz \frac{p_\beta_0(z) \left(1 + \frac{\epsilon \cdot h(z|x)}{p_\beta_0(z)}\right)}{p_\beta_0(z)} \int p(x', y)p_\beta_0(z) \left(1 + \frac{\epsilon \cdot h(z|x')}{p_\beta_0(z)}\right) dx'$$

$$= \int dz \frac{1 + \epsilon \cdot \frac{h(z|x)}{p_\beta_0(z)}}{1 + \epsilon \cdot \frac{h(z|x')p(x')dx'}{p_\beta_0(z)}} \int p(x', y)p_\beta_0(z) \left(1 + \frac{\epsilon \cdot h(z|x')}{p_\beta_0(z)}\right) dx'$$

The $0^{th}$-order term is $\int dz dx'p(x', y)p_\beta_0(z) = p(y)$. The first-order term is

$$\delta p_\beta(z|x) = \epsilon \cdot \int dz dx' \left(h(z|x) + h(z|x') - \int h(z|x')p(x')dx'\right)p(x', y)$$

$$= \epsilon \int dx' \left(\int dz h(z|x) + \int dz h(z|x')\right) - \epsilon \int dx' dx''p(x', y)p(x'') \int dz h(z|x'')$$

$$= 0 - 0$$

$$= 0$$

since we have $\int h(z|x)dz = 0$ for any $x$.

For the second-order term, using $h(z|x) = h^*(x)h_2(z)$ and $C_z = \int \frac{dz}{p_\beta_0(z)} h_2^2(z)$, it is

$$\delta^2 p_\beta(y|x) = \epsilon^2 \int dz \left(\frac{\int h(z|x'')p(x'')dx''}{p_\beta_0(z)}\right)^2 \int p(x', y)p_\beta_0(z)dx'$$

$$- \epsilon^2 \int dz \frac{h(z|x) \int h(z|x'')p(x'')dx''}{(p_\beta_0(z))^2} \int p(x', y)p_\beta_0(z)dx'$$

$$+ \epsilon^2 \int dz \left(h(z|x) - \int h(z|x'')p(x'')dx\right) \int p(x', y)\frac{h(z|x')}{p_\beta_0(z)}dx'$$

$$= \epsilon^2 C_z \left(\int h^*(x'')p(x'')dx''\right)^2 p(y)$$

$$- \epsilon^2 C_z \cdot h^*(x) \int h^*(x'')p(x'')dx''p(y)$$

$$+ \epsilon^2 C_z \cdot h^*(x) \int p(x', y)h^*(x')dx'$$

$$- \epsilon^2 C_z \cdot \int h^*(x'')p(x'')dx \int p(x', y)h^*(x')dx'$$

$$= \epsilon^2 C_z (h^*(x) - \bar{h}_x^*) \left[\left(\int p(x', y)h^*(x')dx'\right) - \bar{h}_x^*p(y)\right]$$

$$= \epsilon^2 C_z (h^*(x) - \bar{h}_x^*) \int p(x', y)\left(h^*(x') - \bar{h}_x^*\right)dx'$$

where $\bar{h}_x^* = \int h^*(x)p(x)dx$. Combining everything, we have up to the second order,

$$p_\beta(y|x) = p(y) + \epsilon^2 C_z (h^*(x) - \bar{h}_x^*) \int p(x, y)(h^*(x) - \bar{h}_x^*)dx$$
I Proof of Theorem 5

Proof. According to Theorem 4, a sufficient condition for \((X,Y)\) to be IB\(_{\beta}\)-learnable is that

\[ X \text{ and } Y \text{ are not independent, and } \beta > \inf_{h(x)} \frac{\mathbb{E}_{x \sim p(x)}[h(x)]^2}{(\mathbb{E}_{x \sim p(x)}[h(x)])^2} - 1 \]  

We can assume a specific form of \(h(x)\), and obtain a (potentially stronger) sufficient condition. Specifically, we let

\[ h(x) = \begin{cases} 1, & x \in \Omega_x \\ 0, & \text{otherwise} \end{cases} \]  

for certain \(\Omega_x \subseteq \mathcal{X}\). Substituting into Eq. (18), we have that a sufficient condition for \((X,Y)\) to be IB\(_{\beta}\)-learnable is

\[ \beta > \inf_{\Omega_x \subseteq \mathcal{X}} \frac{\int_{\Omega_x} p(x | y) dx}{\frac{\int_{\Omega_x} p(x | y) dx}{p(\Omega_x)}} - 1 > 0 \]  

where \(p(\Omega_x) = \int_{x \in \Omega_x} p(x) dx\).

The denominator of Eq. (19) is

\[ \int_{\Omega_x} p(x | y) dx \left( \frac{\int_{\Omega_x} p(x | y) dx}{p(\Omega_x)} - 1 \right)^2 - 1 \]

Using the inequality \(x - 1 \geq \log x\), we have

\[ \mathbb{E}_{y \sim p(y | \Omega_x)} \left[ \frac{p(y | \Omega_x)}{p(y)} - 1 \right] = \mathbb{E}_{y \sim p(y | \Omega_x)} \left[ \log \frac{p(y | \Omega_x)}{p(y)} \right] \geq 0 \]

Both equalities hold iff \(p(y | \Omega_x) = p(y)\), at which the denominator of Eq. (19) is equal to 0 and the expression inside the infimum diverge, which will not contribute to the infimum. Except this scenario, the denominator is greater than 0. Substituting into Eq. (19), we have that a sufficient condition for \((X,Y)\) to be IB\(_{\beta}\)-learnable is

\[ \beta > \inf_{\Omega_x \subseteq \mathcal{X}} \frac{\int_{\Omega_x} p(x | y) dx}{\frac{\int_{\Omega_x} p(x | y) dx}{p(\Omega_x)}} - 1 \]

Since \(\Omega_x\) is a subset of \(\mathcal{X}\), by the definition of \(h(x)\) in Eq. (18), \(h(x)\) is not a constant in the entire \(\mathcal{X}\). Hence the numerator of Eq. (20) is positive. Since its denominator is also positive, we can then neglect the “\(> 0\)”, and obtain the condition in Theorem 5.
Since the \( h(x) \) used in this theorem is a subset of the \( h(x) \) used in Theorem 4, the infimum for Eq. (5) is greater than or equal to the infimum in Eq. (2). Therefore, according to the second statement of Theorem 4, we have that the \((\inf_{\Omega_x \subset X} \beta_0(\Omega_x))^{-1}\) is also a lower bound of the slope for the Pareto frontier of \( I(Y; Z) \) vs. \( I(X; Z) \) curve.

Now we prove that the condition Eq. (5) is invariant to invertible mappings of \( X \). In fact, if \( X' = g(X) \) is a uniquely invertible map (if \( X \) is continuous, \( g \) is additionally required to be continuous), let \( \mathcal{X}' = \{g(x)|x \in \Omega_x\} \), and denote \( g(\Omega_x) \equiv \{g(x)|x \in \Omega_x\} \) for any \( \Omega_x \subset \mathcal{X} \), we have \( p(g(\Omega_x)) = p(\Omega_x) \), and \( p(y|g(\Omega_x)) = p(y|\Omega_x) \). Then for dataset \((X, Y)\), let \( \Omega'_x = g(\Omega_x) \), we have

\[
\frac{1}{\inf_{\Omega_x \subset X} \beta_0(\Omega_x)} = \frac{1}{\inf_{\Omega_x \subset \mathcal{X}'} \beta_0(\Omega'_x)}
\]

Additionally we have \( \mathcal{X}' = g(\mathcal{X}) \). Then

\[
\inf_{\Omega_x \subset \mathcal{X}} \frac{1}{\inf_{\Omega_x \subset \mathcal{X}'} \beta_0(\Omega'_x)} = \inf_{\Omega_x \subset \mathcal{X}'} \frac{1}{\inf_{\Omega_x \subset \mathcal{X}'} \beta_0(\Omega'_x)}
\]

For dataset \((X', Y') = (g(X), Y)\), applying Theorem 5, we have that a sufficient condition for it to be \( \text{IB}_\beta \)-learnable is

\[
\beta > \inf_{\Omega_x \subset \mathcal{X}'} \frac{1}{\inf_{\Omega_x \subset \mathcal{X}'} \beta_0(\Omega'_x)}
\]

where the equality is due to Eq. (22). Comparing with the condition for \( \text{IB}_\beta \)-learnability for \((X, Y)\) (Eq. (5)), we see that they are the same. Therefore, the condition given by Theorem 5 is invariant to invertible mapping of \( X \).

\[\square\]

### J Proof of Corollary 5.1 and Corollary 5.2

#### J.1 Proof of Corollary 5.1

**Proof.** We use Theorem 5. Let \( \Omega_x \) contain all elements \( x \) whose true class is \( y^* \) for some certain \( y^* \), and 0 otherwise. Then we obtain a (potentially stronger) sufficient condition. Since the probability \( p(y|y^*, x) = p(y|y^*) \) is class-conditional, we have

\[
\inf_{\Omega_x \subset \mathcal{X}} \frac{1}{\inf_{\Omega_x \subset \mathcal{X}'} \beta_0(\Omega'_x)} = \inf_{\Omega_x \subset \mathcal{X}} \frac{1}{\inf_{\Omega_x \subset \mathcal{X}'} \beta_0(\Omega'_x)}
\]

By requiring \( \beta > \inf_{y^*} \frac{1}{\inf_{\Omega_x \subset \mathcal{X}} \beta_0(\Omega_x)} \), we obtain a sufficient condition for \( \text{IB}_\beta \) learnability. \[\square\]

#### J.2 Proof of Corollary 5.2

**Proof.** We again use Theorem 5. Since \( Y \) is a deterministic function of \( X \), let \( Y = f(X) \). By the assumption that \( Y \) contains at least one value \( y \) such that its probability \( p(y) > 0 \), we let \( \Omega_x \) contain only \( x \) such that \( f(x) = y \). Substituting into Eq. (5), we have
\[
\frac{1}{p(y)} - 1 \left[ p(y|\Omega_x) \frac{1}{p(y)} - 1 \right] = \frac{1}{p(y)} - 1 \left[ \frac{1}{p(y)} - 1 \right] = 1
\]

Therefore, the sufficient condition becomes \( \beta > 1 \).

**K \ \beta_0, \ hypercontractivity \ coefficient, \ contraction \ coefficient, \ \beta_0[h(x)], \ and \ maximum \ correlation**

In this section, we prove the relations between the IB-Learnability threshold \( \beta_0 \), the hypercontractivity coefficient \( \xi(X;Y) \), the contraction coefficient \( \eta_{KL}(p(y|x), p(x)) \), \( \beta_0[h(x)] \) in Eq. (2), and maximum correlation \( \rho_m(X,Y) \), as follows:

\[
\frac{1}{\beta_0} = \xi(X;Y) = \eta_{KL}(p(y|x), p(x)) \geq \sup_{h(z)} \frac{1}{\beta_0[h(x)]} = \rho_m^2(X;Y)
\]  

(24)

**Proof.** The hypercontractivity coefficient \( \xi \) is defined as (Anantharam et al., 2013):

\[
\xi(X;Y) \equiv \sup_{Z \rightarrow X \rightarrow Y} \frac{I(Y;Z)}{I(X;Z)}
\]

By our definition of IB-learnability, \( (X, Y) \) is IB-Learnable iff there exists \( Z \) obeying the Markov chain \( Z \rightarrow X \rightarrow Y \), such that

\[
I(X;Z) - \beta \cdot I(Y;Z) < 0 \Rightarrow IB_\beta(X,Y;Z) \big|_{p(z|x)=p(z)}
\]

Or equivalently there exists \( Z \) obeying the Markov chain \( Z \rightarrow X \rightarrow Y \) such that

\[
0 < \frac{1}{\beta} < \frac{I(Y;Z)}{I(X;Z)}
\]  

(25)

By Theorem[2] the IB-Learnability region for \( \beta \) is \((\beta_0, +\infty)\), or equivalently the IB-Learnability region for \( 1/\beta \) is

\[
0 < \frac{1}{\beta} < \frac{1}{\beta_0}
\]  

(26)

Comparing Eq. (25) and Eq. (26), we have that

\[
\frac{1}{\beta_0} = \sup_{Z \rightarrow X \rightarrow Y} \frac{I(Y;Z)}{I(X;Z)} = \xi(X;Y)
\]  

(27)

In [Anantharam et al., 2013], the authors prove that
\[ \xi(X; Y) = \eta_{KL}(p(y|x), p(x)) \] (28)

where the contraction coefficient \( \eta_{KL}(p(y|x), p(x)) \) is defined as

\[
\eta_{KL}(p(y|x), p(x)) = \sup_{r(x) \neq p(x)} \frac{\mathbb{D}_{KL}(r(y)||p(y))}{\mathbb{D}_{KL}(r(x)||p(x))}
\]

where \( p(y) = \mathbb{E}_{x \sim p(x)}[p(y|x)] \) and \( r(y) = \mathbb{E}_{x \sim r(x)}[p(y|x)] \). Treating \( p(y|x) \) as a channel, the contraction coefficient measures how much the two distributions \( r(x) \) and \( p(x) \) becomes “nearer” (as measured by the KL-divergence) after passing through the channel.

In [Anantharam et al., 2013], the authors also provide a counterexample to an earlier result by Erkip and Cover (1998) that incorrectly proved \( \xi(X; Y) = \rho_{m}^{2}(X; Y) \). In the specific counterexample [Anantharam et al., 2013] design, \( \xi(X; Y) > \rho_{m}^{2}(X; Y) \).

The maximum correlation is defined as \( \rho_{m}(X; Y) = \max_{f, g} \mathbb{E}[f(X)g(Y)] \) where \( f(X) \) and \( g(Y) \) are real-valued random variables such that \( \mathbb{E}[f(X)] = \mathbb{E}[g(Y)] = 0 \) and \( \mathbb{E}[f^{2}(X)] = \mathbb{E}[g^{2}(Y)] = 1 \) (Hirschfeld, 1935; Gebelein, 1941).

Now we prove \( \xi(X; Y) \geq \rho_{m}^{2}(X; Y) \), based on Theorem 4. To see this, we use the alternate characterization of \( \rho_{m}(X; Y) \) by Rényi (1959):

\[
\rho_{m}^{2}(X; Y) = \max_{f(X)} \mathbb{E}[\{(\mathbb{E}[f(X)|Y])^{2}\}] (29)
\]

Denoting \( \bar{h} = \mathbb{E}_{p(x)}[h(x)] \), we can transform \( \beta_{0}[h(x)] \) in Eq. (2) as follows:

\[
\beta_{0}[h(x)] = \frac{\mathbb{E}_{x \sim p(x)}[h(x)^2] - \mathbb{E}_{x \sim p(x)}[h(x)]^2}{\mathbb{E}_{y \sim p(y)} \left[ (\mathbb{E}_{x \sim p(x|y)}[h(x)])^2 - (\mathbb{E}_{x \sim p(x)}[h(x)])^2 \right]}
\]

\[
= \frac{\mathbb{E}_{x \sim p(x)}[h(x)^2] - \bar{h}^2}{\mathbb{E}_{y \sim p(y)} \left[ (\mathbb{E}_{x \sim p(x|y)}[h(x)])^2 - \bar{h}^2 \right]}
\]

\[
= \frac{\mathbb{E}_{x \sim p(x)}[(h(x) - \bar{h})^2]}{\mathbb{E}_{y \sim p(y)} \left[ (\mathbb{E}_{x \sim p(x|y)}[h(x) - \bar{h}])^2 \right]}
\]

\[
= \frac{1}{\mathbb{E}[\{(\mathbb{E}[f(X)|Y])^{2}\}]}
\]

where we denote \( f(x) = \frac{h(x) - \bar{h}}{(\mathbb{E}_{x \sim p(x)}[(h(x) - \bar{h})^2])^{1/2}} \), so that \( \mathbb{E}[f(X)] = 0 \) and \( \mathbb{E}[f^{2}(X)] = 1 \).

Combined with Eq. (29), we have

\[
\sup_{h(x)} \frac{1}{\beta_{0}[h(x)]} = \rho_{m}^{2}(X; Y) \] (30)

Our Theorem 4 states that

\[
\sup_{h(x)} \frac{1}{\beta_{0}[h(x)]} \leq \frac{1}{\beta_{0}} \leq 1
\] (31)
Combining Eqs. (26), (30) and Eq. (31), we have
\[ \rho_m^2(X; Y) \leq \xi(X; Y) \] (32)

In summary, the relations among the quantities are:
\[ \frac{1}{\tilde{\beta}_0} = \frac{\xi(X; Y) = \eta_{KL}(p(y|x), p(x))}{\sup_{h(x)} \frac{1}{\beta_0[h(x)]}} = \rho_m^2(X; Y) \] (33)

L Experiment Details

We use the Variational Information Bottleneck (VIB) objective from [Aleimi et al. (2016)]. For the synthetic experiment, the latent Z has dimension of 2. The encoder is a neural net with 2 hidden layers, each of which has 128 neurons with ReLU activation. The last layer has linear activation and 4 output neurons; the first two parameterize the mean of a Gaussian and the last two parameterize the log variance. The decoder is a neural net with 1 hidden layer with 128 neurons and ReLU activation. Its last layer has linear activation and outputs the logit for the class labels. It uses a mixture of Gaussian prior with 500 components (for the experiment with class overlap, 256 components), each of which is a 2D Gaussian with learnable mean and log variance, and the weights for the components are also learnable. For the MNIST experiment, the architecture is mostly the same, except the following: (1) for Z, we let it have dimension of 256. For the prior, we use standard Gaussian with diagonal covariance matrix.

For all experiments, we use Adam [Kingma and Ba (2014)] optimizer with default parameters. We do not add any explicit regularization. We use learning rate of $10^{-4}$ and have a learning rate decay of $1 + 0.01 \times \text{epoch}$. We train in total 2000 epochs with mini-batch size of 500.

For estimation of the observed $\beta_0$ in Fig. 3 in the $I(X; Z)$ vs. $\beta_t$ curve ($\beta_t$ denotes the $t^{th}$ $\beta$), we take the mean and standard deviation of $I(X; Z)$ for the lowest 5 $\beta_t$ values, denoting as $\mu_{\beta}, \sigma_{\beta}$ ($I(Y; Z)$ has similar behavior, but since we are minimizing $I(X; Z) - \beta \cdot I(Y; Z)$, the onset of nonzero $I(X; Z)$ is less prone to noise). When $I(X; Z)$ is greater than $\mu_\beta + 3\sigma_\beta$, we regard it as learning a non-trivial representation, and take the average of $\beta_t$ and $\beta_t-1$ as the experimentally estimated onset of learning. We also inspect manually and confirm that it is consistent with human intuition.

For estimating $\beta_0$ using Alg. 1 at step 6 we use the following discrete search algorithm. We fix $i_{\text{left}} = 1$ and gradually narrow down the range $[a, b]$ of $i_{\text{right}}$, starting from $[1, N]$. At each iteration, we set a tentative new range $[a', b']$, where $a' = 0.8a + 0.2b$, $b' = 0.2a + 0.8b$, and calculate $\tilde{\beta}_{0,a'} = \text{Get}(P_{y|x}, P_{y'}, \Omega_{a'})$, $\tilde{\beta}_{0,b'} = \text{Get}(P_{y|x}, P_{y'}, \Omega_{b'})$ where $\Omega_{a'} = \{1, 2, ..., a'\}$ and $\Omega_{b'} = \{1, 2, ..., b'\}$. If $\tilde{\beta}_{0,a'} < \tilde{\beta}_{0,a}$, let $a \leftarrow a'$. If $\tilde{\beta}_{0,b'} < \tilde{\beta}_{0,b}$, let $b \leftarrow b'$. In other words, we narrow down the range of $i_{\text{right}}$ if we find that the $\Omega$ given by the left or right boundary gives a lower $\tilde{\beta}_0$ value. The process stops when both $\tilde{\beta}_{0,a'}$ and $\tilde{\beta}_{0,b'}$ stop improving (which we find always happens when $b' = a' + 1$), and we return the smaller of the final $\tilde{\beta}_{0,a'}$ and $\tilde{\beta}_{0,b'}$ as $\tilde{\beta}_0$.

For estimation of $p(y|x)$ for (2′) Alg. 1 and (3′) $\tilde{\eta}_{KL}$ for both synthetic and MNIST experiments, we use a 3-layer neuron net where each hidden layer has 128 neurons and ReLU activation. The last layer has linear activation. The objective is cross-entropy loss. We use Adam [Kingma and Ba (2014)] optimizer with a learning rate of $10^{-4}$, and train for 100 epochs (after which the validation loss does not go down).

For estimating $\beta_0$ via (3′) $\tilde{\eta}_{KL}$ by the algorithm in [Kim et al. (2017)], we use the code from the GitHub repository provided by the paper\footnote{At https://github.com/wgao9/hypercontractivity} using the same $p(y|x)$ employed for (2′) Alg. 1. Since our datasets are classification tasks, we use $A_{ij} = p(y_j|x_i)/p(y_j)$ instead of the kernel density for estimating matrix $A$; we take the maximum of 10 runs as estimation of $\mu$.\footnote{At https://github.com/wgao9/hypercontractivity}
L.1 Detailed tables for classification with class-conditional noise

In Table L.1 we give the full set of values used for Fig. 3. As the noise rate increases, the true $\beta_0$ increases dramatically. Note that the Observed values are empirical estimates. Corollary 5.1 and Alg. 1 agree almost perfectly when using the true $p(y|x)$. $\hat{\eta}_{KL}$ is somewhat looser, but generally agrees well with the empirical estimates when using the true $p(y|x)$. However, its estimates become much less accurate when $p(y|x)$ is given by a learned neural network trained on the noisy dataset. In contrast, Alg. 1 generally gives much better predictions even when using the estimated $p(y|x)$. Directly optimizing Eq. 2 on the observed data is always an upper bound, although the bound becomes somewhat looser as the noise becomes extreme.

L.2 CIFAR10 Details

We trained a deterministic 28x10 wide resnet [He et al., 2016; Zagoruyko and Komodakis, 2016], using the open source implementation from Cubuk et al. (2018). However, we extended the final 10 dimensional logits of that model through another 3 layer MLP classifier, in order to keep the inference network architecture identical between this model and the VIB models we describe below. During training, we dynamically added label noise according to the class confusion matrix in Tab. L.1. The mean label noise averaged across the 10 classes is 20%. After that model had converged, we used it to estimate $\beta_0$ with Alg. 1. Even with 20% label noise, $\beta_0$ was estimated to be 1.0483.

We then trained 73 different VIB models using the same 28x10 wide resnet architecture for the encoder, parameterizing the mean of a 10-dimensional unit variance Gaussian. Samples from the encoder distribution were fed to the same 3 layer MLP classifier architecture used in the deterministic model. The marginal distributions were mixtures of 500 fully covariate 10-dimensional Gaussians, all parameters of which are trained. The VIB models had $\beta$ ranging from 1.02 to 2.0 by steps of 0.02, plus an extra set ranging from 1.04 to 1.06 by steps of 0.001 to ensure we captured the empirical $\beta_0$ with high precision.

However, this particular VIB architecture does not start learning until $\beta > 2.5$, so none of these models would train as described. Instead, we started them all at $\beta = 100$, and annealed $\beta$ down to the corresponding target over 10,000 training gradient steps. The models continued to train for another 200,000 gradient steps after that. In all cases, the models converged to essentially their final accuracy within 20,000 additional gradient steps after annealing was completed. They were stable over the remaining ~ 180,000 gradient steps.

\footnote{A given architecture trained using maximum likelihood and with no stochastic layers will tend to have higher effective capacity than the same architecture with a stochastic layer that has a fixed but non-trivial variance, even though those two architectures have exactly the same number of learnable parameters.}
Table 1: Full table of values used to generate Fig. 3

| Noise rate | Observed | (1) Corollary | (2) Alg. 1 | (3) $\hat{\eta}_{KL}$ | (4) Eq. 2 | (2') Alg. 1 | (3') $\hat{\eta}_{KL}$ |
|------------|----------|---------------|-------------|------------------------|------------|-------------|------------------------|
| 0.02       | 1.06     | 1.09          | 1.09        | 1.10                   | 1.08       | 1.08        | 1.10                   |
| 0.04       | 1.20     | 1.18          | 1.18        | 1.21                   | 1.18       | 1.19        | 1.20                   |
| 0.06       | 1.26     | 1.29          | 1.29        | 1.33                   | 1.30       | 1.31        | 1.33                   |
| 0.08       | 1.40     | 1.42          | 1.42        | 1.45                   | 1.42       | 1.43        | 1.46                   |
| 0.10       | 1.52     | 1.56          | 1.56        | 1.60                   | 1.55       | 1.58        | 1.60                   |
| 0.12       | 1.70     | 1.73          | 1.73        | 1.78                   | 1.71       | 1.73        | 1.77                   |
| 0.14       | 1.99     | 1.93          | 1.93        | 1.99                   | 1.90       | 1.91        | 1.95                   |
| 0.16       | 2.04     | 2.16          | 2.16        | 2.24                   | 2.15       | 2.15        | 2.16                   |
| 0.18       | 2.41     | 2.44          | 2.44        | 2.49                   | 2.43       | 2.42        | 2.49                   |
| 0.20       | 2.74     | 2.78          | 2.78        | 2.86                   | 2.76       | 2.77        | 2.71                   |
| 0.22       | 3.15     | 3.19          | 3.19        | 3.29                   | 3.19       | 3.21        | 3.29                   |
| 0.24       | 3.75     | 3.70          | 3.70        | 3.83                   | 3.71       | 3.75        | 3.72                   |
| 0.26       | 4.40     | 4.34          | 4.34        | 4.48                   | 4.35       | 4.31        | 4.17                   |
| 0.28       | 5.16     | 5.17          | 5.17        | 5.37                   | 5.12       | 4.98        | 4.55                   |
| 0.30       | 6.34     | 6.25          | 6.25        | 6.49                   | 6.24       | 6.03        | 5.58                   |
| 0.32       | 8.06     | 7.72          | 7.72        | 8.02                   | 7.63       | 7.19        | 7.33                   |
| 0.34       | 9.77     | 9.77          | 9.77        | 10.13                  | 9.74       | 8.95        | 7.37                   |
| 0.36       | 12.58    | 12.76         | 12.76       | 13.21                  | 12.51      | 11.11       | 10.09                  |
| 0.38       | 16.91    | 17.36         | 17.36       | 17.96                  | 16.97      | 14.55       | 10.49                  |
| 0.40       | 24.66    | 25.00         | 25.00       | 25.99                  | 25.01      | 20.36       | 17.27                  |
| 0.42       | 39.08    | 39.06         | 39.06       | 40.85                  | 39.48      | 30.12       | 10.89                  |
| 0.44       | 64.82    | 69.44         | 69.44       | 71.80                  | 76.48      | 51.95       | 21.95                  |
| 0.46       | 163.07   | 156.25        | 156.26      | 161.88                 | 173.15     | 114.57      | 21.47                  |
| 0.48       | 599.45   | 625.00        | 625.00      | 651.47                 | 838.90     | 293.90      | 8.69                   |

Table 2: Class confusion matrix used in CIFAR10 experiments. The value in row $i$, column $j$ means for class $i$, the probability of labeling it as class $j$. The mean confusion across the classes is 20%.

|        | Plane | Auto. | Bird | Cat  | Deer | Dog   | Frog  | Horse | Ship  | Truck |
|--------|-------|-------|------|------|------|-------|-------|-------|-------|-------|
| Plane  | 0.82232 | 0.00238 | 0.021 | 0.00069 | 0.00108 | 0 | 0.00017 | 0.00019 | 0.1473 | 0.00489 |
| Auto.  | 0.00233 | 0.83419 | 0.00009 | 0.00011 | 0 | 0.00001 | 0.00002 | 0 | 0.00946 | 0.15379 |
| Bird   | 0.03139 | 0.00026 | 0.76082 | 0.0095 | 0.07764 | 0.01389 | 0.1031 | 0.00309 | 0.00031 | 0 |
| Cat    | 0.00096 | 0.0001 | 0.00273 | 0.69325 | 0.00557 | 0.28067 | 0.01471 | 0.00191 | 0.00002 | 0.0001 |
| Deer   | 0.00199 | 0 | 0.03866 | 0.00542 | 0.83435 | 0.01273 | 0.02567 | 0.08066 | 0.00052 | 0.00001 |
| Dog    | 0 | 0.00004 | 0.00391 | 0.2498 | 0.00531 | 0.73191 | 0.00477 | 0.00423 | 0.00001 | 0 |
| Frog   | 0.00067 | 0.00008 | 0.06303 | 0.05025 | 0.0337 | 0.00842 | 0.8433 | 0 | 0.00054 | 0 |
| Horse  | 0.00157 | 0.00006 | 0.00649 | 0.00295 | 0.13058 | 0.02287 | 0 | 0.83328 | 0.00023 | 0.00196 |
| Ship   | 0.1288 | 0.01668 | 0.00029 | 0.00002 | 0.00164 | 0.00006 | 0.00027 | 0.00017 | 0.83385 | 0.01822 |
| Truck  | 0.01007 | 0.15107 | 0 | 0.00015 | 0.00001 | 0 | 0.00048 | 0.02549 | 0.81273 |