Nonlinear Information Bottleneck

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Abstract

Information bottleneck [IB] is a technique for extracting information in some 'input' random variable that is relevant for predicting some different 'output' random variable. IB works by encoding the input in a compressed 'bottleneck variable' from which the output can then be accurately decoded. IB can be difficult to compute in practice, and has been mainly developed for two limited cases: (1) discrete random variables with small state spaces, and (2) continuous random variables that are jointly Gaussian distributed (in which case the encoding and decoding maps are linear). We propose a method to perform IB in more general domains. Our approach can be applied to discrete or continuous inputs and outputs, and allows for nonlinear encoding and decoding maps. The method uses a novel upper bound on the IB objective, derived using a non-parametric estimator of mutual information and a variational approximation. We show how to implement the method using neural networks and gradient-based optimization, and demonstrate its performance on the MNIST dataset.

1 Introduction

Imagine that we are provided with two random variables, an 'input' random variable X and an 'output' random variable Y, and that we wish to use X to predict Y. As an example, consider a meteorological scenario, in which X represents recorded data (wind-speed, precipitation, etc.) and Y represents the weather forecast for following days. In many cases, it is useful to extract the information in X that is relevant for predicting Y, e.g., to find the specific (combination of) meteorological features that predict the weather.

This problem is formally considered by the 'information bottleneck' [IB] method [1–3]. Assume that X and Y are jointly distributed according to some P(x,y). IB posits a "bottleneck" variable M which is related to X by the stochastic function P(m|x) called the *encoding map*. Given M, predictions of Y can be made using the *decoding map*,

$$P(y|m) := \frac{P(m,y)}{P(m)} = \frac{\int P(m|x)P(x,y) \, dx}{\int P(m|x)P(x,y') \, dx \, dy'}.$$
 (1)

Note that decoding is done with the assumption that M is conditionally independent of Y given X. This guarantees that any information present in M about Y is extracted from X.

The optimal encoding map is selected by minimizing the IB objective, which balances compression of X and accurate prediction of Y, ¹

$$\mathcal{L}_{\mathrm{IB}} := \beta I(X; M) - I(Y; M).$$

Here $I(\cdot;\cdot)$ is mutual information [6] and $\beta\in[0,1]$ is a parameter that controls the trade-off between compression and prediction². Thus, IB finds the encoding map which minimizes mutual information between X and M (i.e., M maximally compresses X), while maximizing mutual information between M and M (i.e., M optimally predicts M). When M is large, IB will favor maximal compression of M; this can be achieved by making M completely independent of M (thus also from M). When M is small, IB will favor solutions in which M captures maximal information about M. In the limit M0, M1 will recover the minimal sufficient statistics in M2 for M3.

The following example illustrates a possible use-case of IB. Consider a situation where observations of X are made at one physical location while the prediction of Y is made at a different physical location. If these two locations are connected by a low-capacity channel, then it is desirable to transmit as little data as possible between them. For instance, suppose that a remote weather station is making detailed recordings of meteorological data, which are then sent to a central server and used to make probabilistic predictions about weather conditions for the next day. If the channel between the weather station and server has low capacity, then it is important that the information transmitted from the weather station to the server is highly compressed. Minimizing the IB objective amounts to finding a compressed representation (M) of meteorological data (X), which can then be transmitted across a low capacity channel and used to optimally predict future weather (Y). Note that it is also possible to use other measures of compression, such as the Shannon entropy H(M) rather that I(X;M) [8], though such considerations are outside the scope of the present work.

Unfortunately, it is generally intractable to find the encoding maps that optimize the IB objective. This is because it can be very difficult to evaluate the integrals in Eq. (1), as well as the mutual information terms in the IB objective function. For this reason, until now IB has been mainly developed for two limited cases. The first case is where the random variables have a small number of discrete outcomes [1]. There, computation of Eq. (1) and mutual information terms, as well as optimization of $\mathcal{L}_{\mathrm{IB}}$, can be done by explicitly representing all entries of the conditional probability distribution P(m|x). The second case is when X and Y are continuous-valued and jointly Gaussian distributed [4]. Here, the IB optimization problem can be solved analytically, and the resulting optimal encoding and decoding maps are linear.

In this work, we propose a method for performing IB in much more general settings, which we call *nonlinear information bottleneck*, or *nonlinear IB* for short. Our method assumes that M is a continuous-valued random variable, but X and Y can be either discrete (possibly with many states) or continuous, and with any joint distribution. Furthermore, as indicated by the term nonlinear IB, the encoding and decoding maps can be nonlinear.

To implement nonlinear IB, we represent the encoding and decoding maps parametrically, and then minimize an upper bound on the IB objective using gradient-based optimization. Our approach makes use of the following techniques:

- We represent the distributions over X and Y using a finite number of data samples
- We optimize the encoding and decoding maps within some parametric family of densities. The decoding map will not generally equal the integral in Section 3.2, but it can be used to derive a upper bound on the term -I(Y; M) in $\mathcal{L}_{\mathrm{IB}}$
- We use a non-parametric estimator of mutual information to get an upper bound on the term I(X;M) term in $\mathcal{L}_{\mathrm{IB}}$

In the next section, we describe nonlinear IB in detail, and explain its implementation using off-the-shelf neural network software. In Section 4, we demonstrate it on the MNIST dataset of hand-drawn digits.

¹The IB objective is sometimes stated [1, 4, 5] in a different (but equivalent) form, $\mathcal{L}_{\text{IB}} := I(X; M) - \beta I(Y; M)$.

Note that $\beta > 1$ can be ignored, since these values lead only to 'trivial' solutions. This is because M - X - Y form a Markov chain, and the data processing inequality [6] states that $I(X; M) \ge I(Y; M)$. Thus, for $\beta > 1$, the optimal possible value for \mathcal{L}_{IB} is 0, which can be achieved by making M independent of X.

It should be noted that an analogy between IB and neural networks has been previously explored [9]. However, the approach proposed here is not an analogy between IB and neural nets, but rather a direct connection demonstrating that the latter can be used to perform the former. In addition, after an earlier formulation of our approach appeared at the RNN Symposium at the NIPS'16 conference [10], we became aware of three recent papers that similarly propose novel ways of performing IB using upper bounds and gradient-based optimization [11–13]. The major difference between our work and these approaches is in the approximation of the compression term, I(X; Z). This distinction is discussed in more detail in Section 3. In that section, we also relate our approach to other previous work in machine learning.

2 Proposed approach

2.1 Overview

In the following, we use $H(\cdot)$ for Shannon entropy, $I(\cdot;\cdot)$ for mutual information [MI], $D(\cdot||\cdot)$ for Kullback-Leibler [KL] divergence, and $C(\cdot||\cdot)$ for cross-entropy. All information-theoretic quantities are in units of bits, and all logs are base-2.

Let the input X and the output Y be distributed according to some joint distribution Q(x,y), with marginals indicated by Q(y) and Q(x). We assume that we are provided with a 'training dataset' $\mathcal{D} = \{(x_1,y_1),\ldots,(x_N,y_N)\}$, which contains N input-output pairs sampled IID from Q(x,y). Finally, let M indicate the bottleneck variable, with states in \mathbb{R}^d . For simplicity, we assume that X and Y are continuous-valued, though our approach extends immediately to the discrete case (with some integrals replaced by sums).

Let the conditional probability $P_{\theta}(m|x)$, where θ is a vector of parameters, indicate the *encoding map* from input X to the bottleneck variable M. The IB objective, as a function of the encoding map parameters, is written as:

$$\mathcal{L}_{IB}(\theta) := \beta I_{\theta}(X; M) - I_{\theta}(Y; M). \tag{2}$$

In this equation, the first MI term is computed using the joint distribution

$$Q_{\theta}(x,m) := P_{\theta}(m|x) Q(x)$$
,

while the second MI term is computed using the joint distribution

$$Q_{\theta}(y,m) := \int P_{\theta}(m|x) \ Q(x,y) \ dx. \tag{3}$$

We would like to find the encoding map which optimizes the objective,

$$\theta^{\star} = \operatorname*{arg\,min}_{\theta} \mathcal{L}_{IB}(\theta)$$
.

Unfortunately, in many cases this optimization problem is intractable. This is due to the difficulty of computing the integral in Eq. (3) and the MI terms of Eq. (2). However, one can perform approximate IB by minimizing an upper bound on \mathcal{L}_{IB} . Here we derive such an upper bound, and show how it can be optimized.

First, consider some parameterized conditional probability $P_{\phi}(y|m)$ of output given bottleneck, where ϕ is a vector of parameters. For *any* such $P_{\phi}(y|m)$, the non-negativity of KL divergence defines a 'variational' lower-bound on the second MI term in Eq. (2),

$$I_{\theta}(Y; M) = H(Q(Y)) - H(Q_{\theta}(Y|M))$$

$$\geq H(Q(Y)) - H(Q_{\theta}(Y|M)) - D(Q_{\theta}(Y|M) \| P_{\phi}(Y|M))$$

$$= H(Q(Y)) - C(Q_{\theta}(Y|M) \| P_{\phi}(Y|M)) . \tag{5}$$

For this reason, we call $P_{\phi}(y|m)$ the *variational decoding map*. This variational decoding map serves as a tractable approximation to the difficult-to-compute 'optimal' decoding map $Q_{\theta}(y|m)$. This provides us with the following upper bound on the IB objective,

$$\mathcal{L}_{IB}(\theta) \le \beta I_{\theta}(X; M) - H(Q(Y)) + C\left(Q_{\theta}(Y|M) \| P_{\phi}(Y|M)\right). \tag{6}$$

The entropy term H(Q(Y)) does not depend on the parameter values, and is thus irrelevant for optimization. The cross-entropy term can be estimated easily from data, as we show below. Finally, consider minimizing the RHS above as a function of ϕ . Note that this is equivalent to minimizing the KL divergence between $P_{\phi}(y|m)$ and $Q_{\theta}(y|m)$ (Eq. (4)), and will therefore select the $P_{\phi}(y|m)$ which is 'closest' to the optimal decoder map $Q_{\theta}(y|m)$ within the parametric family.

The main remaining challenge is to estimate the first MI term in \mathcal{L}_{IB} , $I_{\theta}(X; M)$. We now provide a tractable upper bound on this MI term that is based on two assumptions.

First, we assume that the encoding map $P_{\theta}(m|x)$ is the sum of a deterministic differentiable function $f_{\theta}(x)$ and Gaussian noise with covariance matrix $\sigma^2 \mathbf{I}$,

$$P_{\theta}(m|x) := p_{\text{normal}}(m; f_{\theta}(x), \sigma^{2}\mathbf{I}), \tag{7}$$

where $p_{\text{normal}}(\cdot; \mu, \Sigma)$ is the p.d.f. of a multivariate Gaussian with mean μ and covariance matrix Σ . Note that σ is considered as one of the parameters in θ , and hence is optimized.

The second assumption we make is that the distribution of $f_{\theta}(X)$ can be approximated as a finite mixture of Gaussians [MoG]. Specifically, this MoG contains one Gaussian component for each training data point i = 1..N in \mathcal{D} with mean $f_{\theta}(x_i)$ and covariance matrix $\eta^2 \mathbf{I}$. The parameter η^2 is chosen using cross-validation to maximize the leave-one-out log likelihood of the training data [14],

$$\eta(\theta) = \arg\max_{s} \sum_{i} \log \left(\frac{1}{N-1} \sum_{j \neq i} \left(\frac{1}{(2\pi s^2)^{d/2}} \exp\left(-\frac{\|f_{\theta}(x_i) - f_{\theta}(x_j)\|_2^2}{2s^2} \right) \right) \right), \quad (8)$$

where we've made the dependence of η on θ explicit. Under mild assumptions, MoG models converge to the true distribution as the size of the training dataset grows [15].

To summarize, we've assumed that the distribution of $f_{\theta}(X)$ is a MoG, with each component having covariance $\eta^2(\theta)\mathbf{I}$. M is then computed by adding Gaussian noise with covariance $\sigma^2\mathbf{I}$ to $f_{\theta}(X)$ (Eq. (7)). This means that M is distributed as a MoG, with each component having covariance $(\eta^2(\theta) + \sigma^2)\mathbf{I}$,

$$p(M = m) := \frac{1}{N} \sum_{i=1}^{N} p_{\text{normal}}(m; f_{\theta}(x_i), (\eta^2(\theta) + \sigma^2)\mathbf{I}).$$

We now propose the following upper bound on the mutual information between X and M:

$$I_{\theta}(X;M) = H(M) - H(P_{\theta}(M|X)) \le \hat{I}_{\theta}^{\mathcal{D}}, \tag{9}$$

where $\hat{I}_{\theta}^{\mathcal{D}}$ is defined as

$$\hat{I}_{\theta}^{\mathcal{D}} := -\frac{1}{N} \sum_{i} \log \frac{1}{N} \sum_{j} \exp\left(-\frac{1}{2} \frac{\|f_{\theta}(x_{i}) - f_{\theta}(x_{j})\|_{2}^{2}}{\eta(\theta)^{2} + \sigma^{2}}\right) - \frac{d}{2} \log \frac{\sigma^{2}}{\eta(\theta)^{2} + \sigma^{2}}, \quad (10)$$

and (as before) d is the dimensionality of M. We use two techniques to derive this upper bound. First, we note that $H(P_{\theta}(M|X))$ is the entropy of a multivariate Gaussian with covariance $\sigma^2 \mathbf{I}$, which has a simple closed-form expression [6]. Second, we bound H(M) using a non-parametric upper bound on the entropy of a mixture, described in detail in [16]. Combining these two leads to $\hat{I}^{\mathcal{D}}_{\theta}$ [16]. This bound can be understood as a 'corrected' kernel-based MI-estimator.

Note that $\hat{I}_{\theta}^{\mathcal{D}}$ is a differentiable function of θ , and thus can be optimized using gradient-based methods. Furthermore, as shown in [16], when f_{θ} maps the dataset into several well-separated clusters this bound becomes an exact estimate of the empirical MI (a commonly-encountered solution to the optimization problem posed here).

Combining Eq. (6) and Eq. (9) provides a tractable upper bound,

$$\mathcal{L}_{\mathrm{IB}}(\theta) \leq \hat{\mathcal{L}}_{\mathrm{IB}}(\theta, \phi) := \beta \hat{I}_{\theta}^{\mathcal{D}} + C\left(Q_{\theta}(Y|M) \| P_{\phi}(Y|M)\right) + \mathrm{const}$$

where H(Q(Y)) has been absorbed into 'const'. Nonlinear IB seeks parameter values that minimize this upper bound,

$$\theta^{\star}, \phi^{\star} = \underset{\theta, \phi}{\arg\min} \, \hat{\mathcal{L}}_{IB}(\theta, \phi) \,. \tag{11}$$

2.2 Implementation

We show that the nonlinear IB optimization problem (Eq. (11)) can be carried out using a finite-sized training set and neural network (NN) optimization techniques.

The encoding map $P_{\theta}(m|x)$, as specified by Eq. (7), is computed in the following way: first, several NN layers implement the (possibly nonlinear) deterministic function $f_{\theta}(x)$. The output of these layers is then added to zero-centered Gaussian noise with covariance $\sigma^2 \mathbf{I}$, which becomes the state of the *bottleneck layer*. The parameter vector θ specifies all relevant connection weights and biases of these layers, as well as the noise variance σ . Note that due to the presence of noise, the neural network is stochastic: even with parameters held constant, different states of the bottleneck layer would be sampled during different NN evaluations.

The decoding map $P_{\phi}(y|m)$ is also computed by the neural network. First, the bottleneck layer states are passed through several deterministic layers of the network, whose parameters (connections and biases) are specified by the vector ϕ . The log decoding probability $\log P_{\phi}(y|m)$ is then computed using an appropriately-chosen neural network cost function (e.g., squared-error for continuous Y, cross-entropy for discrete Y [17]).

Given a finite training dataset $\mathcal{D} = \{(x_1, y_1), \dots, (x_N, y_N)\}$, the optimal encoding and decoding maps are determined by minimizing

$$\hat{\mathcal{L}}_{\mathrm{IB}}(\theta, \phi) \approx \beta \hat{I}_{\theta}^{\mathcal{D}} - \frac{1}{N} \sum_{i=1}^{N} \log P_{\phi}(y_i | m_i),$$

where m_i is sampled from $P_{\theta}(m|x_i)$, and $\hat{I}_{\theta}^{\mathcal{D}}$ is specified in Eq. (10). Note that this finite sample approximation converges to $\hat{\mathcal{L}}_{\text{IB}}$ as the training dataset size $N \to \infty$.

All terms in the above approximation are differentiable. Thus, a local optimum of $\hat{\mathcal{L}}_{\mathrm{IB}}$ can be found by gradient-descent. However, there are several important caveats. In practice we compute the gradient of $\sum_{i=1}^N \log P_\phi(y_i|m_i)$ using stochastic gradient descent (SGD) using mini-batches of size n_{SGD} . The gradient of the term $\hat{I}^{\mathcal{D}}_{\theta}$ is also computed using SGD, but using different mini-batches of size n_{MI} . Generally, we choose $n_{\mathrm{MI}} > n_{\mathrm{SGD}}$, because having a larger n_{MI} significantly improves the estimate of mutual information in high-dimensional spaces (i.e., large d), while having smaller n_{SGD} improves generalization performance [18]. In addition, note that the 'width' of the MI estimator, η , is continually updated as the optimization proceeds.

In practice, we carry out the following procedure:

- 1. A mini-batch \mathcal{D}_{SGD} of size n_{SGD} and a mini-batch \mathcal{D}_{MI} of size n_{MI} are randomly sampled from the training dataset \mathcal{D} .
- 2. Holding θ and ϕ fixed, an optimizer selects the best value of η , according to Eq. (8) computed over \mathcal{D}_{MI} .
- 3. For each input x_i in \mathcal{D}_{SGD} , a value of m_i is sampled from $P_{\theta}(m|x_i)$. These samples are used to compute the stochastic gradient of $-\sum_i \log P_{\phi}(y_i|m_i)$ w.r.t. to θ and ϕ . To this is added β times the stochastic gradient of $\hat{I}_{\theta}^{\mathcal{D}}$ w.r.t. to θ , computed over \mathcal{D}_{MI} . A step is taken in the direction of this combined gradient.
- 4. The process repeats.

Note that training is more effective when σ^2 is initially small, so that information about the gradient of $-\sum_i \log P_{\phi}(y_i|m_i)$ is not completely destroyed by noise during early training.

3 Relation to existing approaches

3.1 Neural networks and Kernel Density Entropy Estimates

One important idea in our approach is using a differentiable, kernel-based estimator of mutual information, $\hat{I}_{\theta}^{\mathcal{D}}$. See [19–23] for related ideas about using neural networks to optimize non-parametric estimates of information-theoretic functions. This technique can also be related the estimation of

held-out data likelihood in deep learning models using kernel-based estimators (e.g., [24]). However, in these approaches, held-out data likelihood is estimated only once, as a diagnostic measure once learning is complete. We propose to instead directly optimize these non-parametric estimators.

3.2 Variational IB

After the appearance of an earlier formulation of this approach [10], we became aware of three recent papers that also propose methods for performing IB for continuous, possibly non-Gaussian random variables [11–13]. In this section, we compare these papers with the approach presented here.

As in our work, these papers propose tractable upper bounds on the \mathcal{L}_{IB} objective function which can be optimized using neural-network-based methods. They employ the same variational bound for the MI term $I_{\theta}(Y; M)$ (Eq. (5)) as we do,

$$I_{\theta}(Y;M) \geq H(Q(Y)) - C\left(Q_{\theta}(Y|M) \| P_{\phi}(Y|M)\right),$$

where $P_{\phi}(y|m)$ is the variational decoding map. These methods (and ours) differ, however, in their treatment of $I_{\theta}(X;M)$. These methods bound $I_{\theta}(X;M)$ using a parametric marginal distribution over the bottleneck variable $R_{\alpha}(m)$, where α is some vector of parameters. This gives a variational bound for $I_{\theta}(X;M)$,

$$I_{\theta}(X; M) = H(Q_{\theta}(M)) - H(P_{\theta}(M|X))$$

$$\leq C(Q_{\theta}(M) || R_{\alpha}(M)) - H(P_{\theta}(M|X))$$

$$= D(P_{\theta}(M|X) || R_{\alpha}(M)).$$
(12)

Combining leads to the following variational bound for \mathcal{L}_{IB} ,

$$\mathcal{L}_{IB} \le \mathcal{L}_{VIB} := \beta D(P_{\theta}(M|X) || R_{\alpha}(M)) + C\left(Q_{\theta}(Y|M) || P_{\phi}(Y|M)\right) + \text{const.}$$
 (13)

The three aforementioned papers differ in how they define the approximate marginal distribution $R_{\alpha}(m)$. In [12], $R_{\alpha}(m)$ is a standard multivariate normal distribution, $R(m) := p_{\text{normal}}(m|0, \mathbf{I})$. In [11], $R_{\alpha}(m)$ is a product of Student-t distributions, $R_{\alpha}(m) := \prod_{i=1}^d p_{\text{Student}}(m|0, w_i^2, \nu_i)$, where w_i^2 and ν_i specify the scale and shape parameters of the i-th dimension. The parameters w_i and ν_i are encoded in α and optimized during learning, in this way tightening the bound in Eq. (12). In [13], two approximating distributions are considered: the improper log-uniform, $R(\log m) := c$, and the log-normal, $R(\log m) := p_{\text{normal}}(\mu, \sigma^2)$. Additionally, the encoding map consists of a deterministic function with multiplicative noise. Finally, in [11, 12], the encoding map $P_{\theta}(m|x)$ is treated as deterministic function plus Gaussian noise, similarly to how it is treated here.

In a sense, our proposed methodology also approximates the distribution over the bottleneck variable. However, rather than use a parametric variational distribution, our approximation is based on a *non-parametric* kernel-based estimator, and as mentioned, the estimate converges to the true $Q_{\theta}(M)$ in the large sample limit.

These alternative methods have potential advantages and disadvantages compared to our approach. On one hand, they are more computationally efficient: our non-parametric estimator of $I_{\theta}(X;M)$ requires $O(n^2)$ operations per SGD batch (where n is the size of the mini-batch), while the variational bound of Eq. (12) requires O(n) operations. On the other hand, our non-parametric estimator is expected to give a better estimate of the MI $I_{\theta}(X;M)$. In fact, in [16], we show that our bound is tight, or near tight, in many cases of interest. This improved estimate of the mutual information will improve the optimization of the compression term (i.e., $I_{\theta}(X;M)$), and may lead to significant performance improvement in some cases.

A thorough comparison of these different approach remains for future work (see also the Results section).

3.3 Auto-encoders

The central idea of IB is to find a mapping from inputs to outputs while using a "compressed" intermediate representation. This idea has several precedents in the machine learning literature.

One important example is work on *auto-encoders*. Auto-encoders are machine learning architectures that attempt to reconstruct a copy of the input X, while using some restricted 'intermediate representations' (typically encoded in the activity of a hidden layer in a neural network). Auto-encoders

are conceptually similar to IB, and can be understood as optimizing the encoding map $P_{\theta}(m|x)$ and decoding map $P_{\phi}(y|m)$ where X=Y (i.e., input data is compressed into an intermediate representation, from which the same input data can then be uncompressed). Auto-encoders may also regularize the encoding map, e.g., by placing information-theoretic penalties on the coding length of hidden layer activity [25, 26]. This idea has also been explored in a supervised learning scenario in [27]. In that work, however, hidden layer states were treated as discrete-valued, limiting the flexibility and information capacity of hidden representations. More recently, denoising auto-encoders [28] have attracted attention. Denoising auto-encoders constrain the amount of information between input and hidden layers by injecting noise into the hidden layer activity, somewhat similar to our noisy mapping between input and bottleneck layers. Existing work on auto-encoders has considered either penalizing hidden layer coding length or injecting noise into the map, rather than combing the two as we do here. Because of this, denoising auto-encoders do not have a notion of "optimal" noise level on the training data (since less noise will always improve prediction error on the training data), and thus cannot directly adapt the noise level.

Variational auto-encoders [29] [VAE] are another recent machine-learning architecture. VAEs use neural network techniques to perform unsupervised learning, i.e., to learn generative models from data. VAE postulate a 'latent variable' M (in our language, a bottleneck variable) distributed according to some $R_{\alpha}(m)$, where α indicates parameters. Samples of the latent variable are then mapped to observed data space X according to

$$P_{\alpha,\phi}(x) = \int P_{\phi}(x|m)R_{\alpha}(m) \ dm \,,$$

where P_{ϕ} is a conditional probability density parameterized by ϕ . Using our terminology, P_{ϕ} can be understood as a decoding map given the assumption that X = Y.

Given a dataset $\mathcal{D} = \{x_1, \dots, x_N\}$, VAE attempts to choose parameters ϕ and α that maximize the marginal likelihood $P_{\alpha,\phi}$ of the samples in \mathcal{D} . However, computing the marginal likelihood of data is generally intractable. For this reason, VAE minimizes the following upper bound on the negative log likelihood of the data,

$$\mathcal{L}_{VAE}(\theta, \phi, \alpha) = D(P_{\theta}(M|X)||R_{\alpha}(M)) + C(Q_{\theta}(X|M)||P_{\phi}(X|M)),$$

where $Q_{\theta}(x|m)$ is the Bayesian inverse of $P_{\theta}(m|x)$,

$$Q_{\theta}(x|m) := \frac{P_{\theta}(m|x)Q(x)}{\int P_{\theta}(m|x')Q(x') dx'}.$$

As was observed [12, 13], this objective is identical to \mathcal{L}_{VIB} (Eq. (13)), assuming $\beta = 1$ and X = Y.

Interestingly, by working back through Eq. (12), one can show that the optimal $R_{\alpha}(m)$ for this objective is

$$R^{\star}(m) = \int P_{\theta}(m|x) Q(x) dx.$$

Fixing this optimal $R^{\star}(m)$, the VAE upper bound becomes

$$\mathcal{L}_{\text{VAE}}(\theta, \phi) = I(X; M) + C(Q_{\theta}(X|M) || P_{\phi}(X|M))$$

$$\leq \hat{I}_{\theta}^{\mathcal{D}} + C(Q_{\theta}(X|M) || P_{\phi}(X|M)),$$

where in the second line we've used the estimator used in nonlinear IB (Eq. (10)).

Thus, the method proposed in this work can also be used to provide a tractable upper bound on the negative log likelihood in VAE. This suggests that our approach may offer a novel way of learning VAE-based generative models from data. Exploring its potential in this domain remains for future work.

4 Results

We demonstrate our approach on the MNIST dataset of images of hand-drawn digits. This dataset contains a set of 60,000 training images and 10,000 testing images. Each image is 28-by-28 pixels, and is classified into one of 10 classes corresponding to the digit identity. $X \in \mathbb{R}^{784}$ is defined to be the vector of the 28-by-28 pixel values, and $Y \in \{1..10\}$ is defined to be the class label.

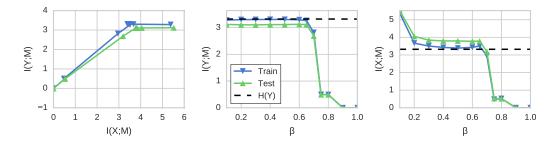


Figure 1: Values of β versus estimates of I(X; M) and I(Y; M) on the MNIST dataset. Dashed line indicates $H(Y) = \log 10$.

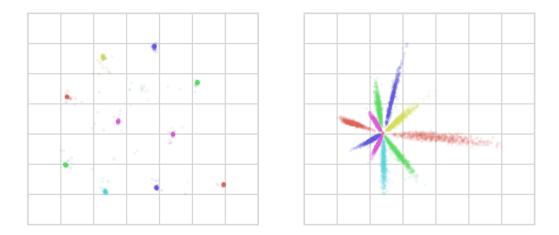


Figure 2: Bottleneck layer activity (without noise). Left: nonlinear IB ($\beta=0.4$); Right: regular supervised learning ($\beta=0$).

The encoding function f_{θ} was implemented using three NN layers: the first layer consisted of 800 Rectified-Linear [relu] units, the second layer consisted of 800 relu units, and the third layer consisted of 20 linear units. The state of the bottleneck variable $M \in \mathbb{R}^{20}$ corresponded to the activity of this third layer plus noise. The decoding map p_{ϕ} was implemented using two neural-network layers: a layer of 800 relu units, followed by a layer of 10 softmax units, and then the cross-entropy error function.

The optimization was performed using an off-the-shelf deep learning framework [30–32]. The Adam [33] optimizer was used, and training was run for 200 epochs. The initial learning rate was 0.001 and dropped 60% every 10 epochs. Mini-batch sizes of $n_{\rm SGD}=128$ and $n_{\rm MI}=1000$ were used. All relevant code is available at https://github.com/artemyk/nonlinearIB.

Fig. 1 show values of β versus estimates of I(X;M) and I(Y;M) on the MNIST dataset, for both training and testing datasets. We also plot $H(Y) = \log 10$ as a dotted line (H(Y)) is an upper bound on the possible MI term I(Y;M), and a lower bound on the minimal I(X;M) necessary for completely-accurate prediction of Y from M). For these plots, I(X;M) was estimated using Eq. (10), while I(Y;M) was estimated using the lower bound of Eq. (5),

$$I(Y; M) \ge H(Y) - C(Q_{\theta}(Y|M) || P_{\phi}(Y|M)).$$

As can be seen from the figure, our methods permits us to trade off between maximal information about Y versus maximal compression of X by varying β .

Additional insight is provided by considering the intermediate representations uncovered by nonlinear IB (with $\beta=0.4$) versus regular supervised learning (with $\beta=0$). To visualize these intermediate representations, we optimized a slightly different network: here, f_{θ} was implemented by a stack of three NN layers: the first layer and second layers again consisted of 800 relu units, while the third

layer consisted of two linear units. The state of the bottleneck variable $M \in \mathbb{R}^2$ corresponded to the activity of this third layer plus noise. This configuration makes the neural network map the high-dimensional input space of images into a two-dimensional, easily-visualizable representation. The decoding map consisted of an 800-node layer of relu units and a 10-node softmax layer, as before.

Fig. 2 visualizes states of the 2-dimensional bottleneck layer (before adding noise) for a subsample of the training dataset, with colors indicating digit identity. This is shown both for nonlinear IB ($\beta=0.4$) and regular supervised learning ($\beta=0$) training. Both methods successfully separate different digits into different regions of the bottleneck layer state space. However, with regular supervised learning (right), images of each digit are mapped onto a large 'swath' of activity, and bottleneck states carry information about input vectors beyond digit identity. On the other hand, nonlinear IB (left) tends to map images of each digit into a separate and very tight cluster. These bottleneck states carry almost no information about input vectors beyond digit identity.

Finally, it is of interest to compare our approach with variational methods described in Section 3.2. However, the method described in [12] had no publically-available code provided. We developed our own implementation of this method (available at https://github.com/artemyk/nonlinearIB), but could not replicate replicate the published results [12], even after extensive private communication with the authors. Theoretical and numerical comparisons with such variational methods thus remain an important area of investigation for the future.

5 Conclusion

We propose 'nonlinear IB', a method for performing information bottleneck [IB] in novel domains. We assume that the bottleneck variable is continuous. However, unlike previous approaches, the input and output variables can be either discrete or continuous, can be distributed in arbitrary (e.g., non-Gaussian) ways, and the encoding and decoding maps can be nonlinear. Our method is based on a new tractable upper bound on the IB objective. This upper bound can be optimized using gradient-based techniques applied to training data. We show how to implement our method using an off-the-shelf neural network package. We then demonstrate it on the MNIST dataset of handwritten digits, showing that it uncovers very different intermediate representations than those uncovered by traditional supervised learning.

Note that we have discussed nonlinear IB as a technique for finding compressed representations of the input. The method may also be used an information-theoretic regularizer, i.e., as a way to penalize over-fitting and improve generalization performance. Exploring its efficacy in this domain remains for future work.

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