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# Tighter Bounds on the Information Bottleneck with Application to Deep Learning

Anonymous submission

#### **Abstract**

Deep Neural Nets (DNNs) learn latent representations induced by their downstream task, objective function and other parameters. The quality of their data modeling affects the DNN's ability to generalize and the coherence of the emerging latent space. The Information Bottleneck, IB, offers an optimal information theoretic framework for data modeling, however, it is intractable in most settings. In recent years attempts were made to combine deep learning with the IB both for optimization and for the interpretation of DNNs. VAE inspired variational approximations became a popular method to approximate bounds on the required mutual information computations. This work introduces a new tractable variational upper bound for the IB functional which is tighter than previous bounds. When used as an objective function it enhances the performance of previous IB-inspired DNNs in terms of test accuracy while providing similar or superior robustness to adversarial attacks. These improvements in performance, induced by a tighter bound, strengthen the cause for the IB and it's variational approximations as a framework for better representation learning. Furthermore, we present practitioners with a simple method to substantially increase adversarial robustness of any classifier DNN while suffering only a slight decrease in performance over unseen data.

# 1. Introduction

In recent years deep neural nets have gained increasing popularity in different learning tasks. Their ability to approximate complicated functions has revolutionized many computational fields. Despite the great achievements, it is still postulated that the current networks are prone to overfit the training data (Ying, 2019), may be considerably uncalibrated (Guo et al., 2017) and are susceptible to adversarial attacks (Goodfellow et al., 2015). A question emerges regarding the extraction of an optimal representation for all data points from our restricted set of training

examples. Classic information theory provides tools to optimize compression and transmission of data, but it does not provide methods to gauge the relevance of the compressed signal to downstream tasks. Methods such as rate distortion (Blahut, 1972) regard all information as equal, not taking into account which information is more relevant without constructing complex distortion functions. To resolve these limitations, the Information Bottleneck, IB (Tishby et al., 1999), defines an information theoretic limit for the rate distortion ratio of any learning task given a Lagrangian hyper parameter  $\beta$  controlling the tradeoff between the rate and the distortion. Optimizing a learning task using the IB objective results in an encoding with optimal rate distortion ratio for a downstream task, over a chosen Lagrangian  $\beta$  and for a mutual information distortion function. Computing the IB requires mutual information calculations which are tractable in discrete settings and for some specific continuous distributions. Adopting the IB framework for DNNs requires computing mutual information for unknown distributions and has no analytic solution. However, recent work approximated tractable upper bounds for the IB functional in DNN settings using variational approximations. Variational auto encoders (Kingma & Welling, 2014) use stochastic DNNs to approximate intractable and unknown distributions. Assuming a latent variable model the marginal  $p(x) = \int p(x|z)p(z)dz$  (Where X is an observed variable and Z is unobserved) can be approximated using a chosen variational distribution optimized to fit the training data. This optimization is possible using Stochastic Gradient Descent (SGD) and the 'reparameterization trick' as elaborated in Section 2.3. Similarly to VAEs Alemi et al. (2017) proposed using stochastic DNNs as variational approximations for a latent model thus making possible the computations of upper bounds for mutual information between the DNN's input, output and hidden layers. A proposed optimization method called VIB - 'Deep Variational Information Bottleneck' derives an upper bound for the IB objective and minimizes it's approximation using Monte Carlo sampling over training data. Alemi et al. (2017) found that replacing a DNN's deterministic classifier layer with a stochastic layer optimized with the VIB objective results in a slight decrease in test set accuracy but a significant increase in robustness to adversarial attacks in complicated classification tasks. Similar behavior is demonstrated in the current work as shown

in Section 4.

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The case for the IB functional, and it's variational approximations, as a theoretical limit for optimal representation relies on three assumptions: (1) It suffices to optimize the mutual information metric to optimize a model's performance; (2) Forgetting more information about the input while keeping the same information about the output induces better generalization over unseen data; (3) Mutual information between the input, output and latent representation can be either computed or approximated to a desired level of accuracy.

In this study, we adopt the same information theoretic and variational approach used previously. The work begins by deriving an upper bound for the IB functional. We then employ a tractable variational approximation for this bound, named VUB - 'Variational Upper Bound' and show that it is a tighter bound on IB than VIB. We proceed to show empirical evidence that VUB substantially increases test accuracy over VIB while providing similar or superior robustness to adversarial attacks across several challenging tasks and modalities. Finally, we discuss these effects in the context of previous work on IB and other DNN regularization techniques. The conclusion drawn is that while more mutual information between encoding and output does not necessarily improve classification, and more compressed encoding does not always enhance regularization (Amjad & Geiger, 2020), the application of IB approximations as objectives to DNNs empirically improves regularization, suggesting better data modeling. This notion contributes for the adaptation of the IB, and it's variational approximations, as an objective to learning tasks and as a theoretic framework to gauge and explain regularization.

In addition, we demonstrate that VUB can be easily adapted to any classifier DNN, including transformer based NLP classifiers, to substantially increase robustness to adversarial attacks while only slightly decreasing test accuracy.

#### 1.1. Preliminaries

The following literature review and derivations refer to information theory and variational approximations. A preliminary mutual ground and notation follows:

We denote random variables with upper cased letters X,Y, and their realizations in lower case x,y. Denote discrete Probability Mass Functions (PMFs) with an upper case P(X) and continuous Probability Density Functions (PDFs) with a lower case p(x). Hat notation denotes empirical measurements.

Let X, Y be two observed random variables (RVs) with unknown distributions  $p^*(x), p^*(y)$  that we aim to model. Assume X, Y are governed by some unknown underlying process with a joint probability distribution  $p^*(x, y)$ . We

can attempt to approximate these distributions using a model  $p_{\theta}$  with parameters  $\theta$  such that for generative tasks  $p_{\theta}(x) \approx$  $p^*(x)$  and for discriminative tasks  $p_{\theta}(y|x) \approx p^*(y|x)$ , using a dataset  $S = \{(x_1, y_1), ..., (x_N, y_N)\}$  to fit our model. One can also assume the existence of an additional unobserved RV  $Z \sim p^*(z)$  that influences or generates the observed RVs X, Y. Since Z is unobserved it is absent from the dataset S and so cannot be modeled directly. Denote  $\int p_{\theta}(x|z)p_{\theta}(z)dz$  the marginal,  $p_{\theta}(z)$  the prior as it is not conditioned over any other RV, and  $p_{\theta}(z|x)$  the posterior following Bayes' rule. Latent models are frequently used for creating variational bounds on mutual information as they make good approximations for  $p^*(x)$  due to their high expressivity (Kingma & Welling, 2019), as is demonstrated in Section 2.3. Deep neural nets, or DNNs, are a powerful tool to approximate complicated functions such as modeling  $p_{\theta}(y|x)$  or  $p_{\theta}(x)$ . When choosing a DNN to approximate a latent model we encounter a problem as the marginal integral  $p_{\theta}(x) = \int p_{\theta}(x, z) dz$  doesn't have an analytic solution and hence not optimizable over gradient descent (Kingma & Welling, 2019). This intractability can be overcome by using a tractable parametric variational encoder  $q_{\phi}(z|x)$  to approximate the posterior  $p_{\theta}(z|x)$  such that  $q_{\phi}(z|x) \approx p_{\theta}(z|x)$ , and estimate  $p_{\theta}(x, z)$  or  $p_{\theta}(x, z|y)$  using Monte Carlo sampling from the dataset S during optimization.

In this work information theoretic functions share the same notation for discrete and continuous settings and are denoted as follows:

$$\begin{array}{ll} \text{Entropy} & H_p(X) = -\int p(x)log\left(p(x)\right)dx \\ \text{Cross} & CE(P,Q) = \\ \text{entropy} & -\int p(x)log\left(q(x)\right)dx \\ \text{KL} & D_{KL}\left(P\Big|\Big|Q\right) = \\ & \int p(x)log\left(\frac{p(x)}{q(x)}\right)dx \\ \text{Mutual} & I(X;Y) = \\ & \inf \text{ormation} & \int \int p(x,y)log\left(\frac{p(x,y)}{p(x)p(y)}\right)dxdy \end{array}$$

# 2. Related work

#### 2.1. IB and it's analytic solutions

Classic information theory offers rate-distortion (Blahut, 1972) to mitigate signal loss during compression. Rate being the signal's compression measured by mutual information between input and output signals, and distortion a chosen task-specific function. The Information Bottleneck method extends rate-distortion by replacing the tailored distortion functions with mutual information over a target distribution. This allows optimizing a signal's compression to any chosen downstream task. Denote X the source signal, Z it's encoding and Y the target signal for some

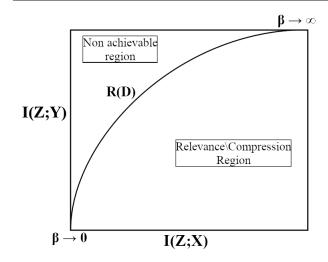


Figure 1. The information plane and curve - rate distortion ratio over  $\beta$ . Adapted from (Slonim, 2002). At  $\beta=0$ , representation is compressed but uninformative (maximal compression), at  $\beta \to \infty$  it's informative but potentially overfitted (maximal information).

specific downstream task. Let T be a positive minimal threshold for the desired distortion and assume a latent variable model with the Markov chain  $Z \leftrightarrow X \leftrightarrow Y$  and define the distortion function as mutual information between encoding and downstream task. We seek an optimal encoding  $Z: \min_{P(Z|X)} I(X;Z)$  subject to  $I(Z;Y) \geq T$ . This constrained problem can be implicitly optimized by minimizing

strained problem can be implicitly optimized by minimizing the functional  $L_{P(Z|X)} = I(Z;X) - \beta I(Z;Y)$  over the Lagrangian  $\beta$ , the first term being rate and the second distortion. The optimal solution is a function of  $\beta$  and was named 'the information curve' as shown in Figure 1.

The IB functional is only tractable when mutual information can be computed and was demonstrated by Tishby et al. (1999) for soft clustering tasks over a discrete and known distribution  $P^*(x,y)$ . Chechik et al. (2003) extended IB for gaussian distributions and Painsky & Tishby (2017) offered a limited linear approximation of IB for any distribution.

# 2.2. IB and deep learning

Tishby & Zaslavsky (2015) proposed an IB interpretation of DNNs regarding them as Markov cascades of intermediate representations between hidden layers. Neural architecture and dataset cardinality are theoretically sufficient to compute the optimal rate distortion of a DNN on the information curve. This suggests a model *complexity gap* between the achieved and optimal IB compression rate for that setting, and it is hypothesized that bridging this gap will result in optimal generalization. Shwartz-Ziv & Tishby (2017) visualized and analyzed the information plane behavior of DNNs over a toy problem with a known joint distribution.

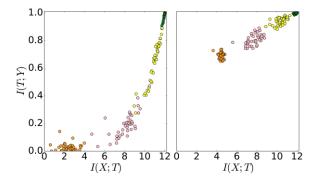


Figure 2. Information plane scatters of different DNN layers (colors) in 50 randomized networks. From Shwartz-Ziv & Tishby (2017). Left are initial weights, Right are at 400 epochs. I(T;Y), I(X;T) are analogous to I(Z;Y), I(X;Z) in the current study. We believe to be the first to demonstrate similar information plane behavior on real-world problems as shown in Figure 3.

Mutual information of the different layers was estimated and used to analyze the training process. SGD exhibited two separate and sequential behaviors during training: A short empirical error minimization phase (ERM) characterized by larger gradient norms and a rapid decrease in distortion, followed by a long compression phase with smaller gradient norms and an increase in rate until convergence to an optimal IB limit as demonstrated in Figure 2.

Amjad & Geiger (2020) pointed out three flaws in the usage of the IB functional as an objective for deterministic DNN classifiers: (1) When data X is absolutely continuous the mutual information term I(X;Z) is infinite; (2) When data X is discrete the IB functional is a piecewise constant function of the parameters, making it's SGD optimization difficult or impossible; (3) Equivalent representations might yield the same IB loss while one achieved much better classification rate than the other. These discrepancies were attributed to to mutual information's invariance to invertible transformations and the absence of the decision function in the objective.

# 2.3. Variational approximations to the IB objective

Kingma & Welling (2014) introduced the variational auto encoder - a stochastic generative DNN. An unobserved RV Z is assumed to generate evidence X,Y and the true probability  $p^*(x)$  can be modeled using a parametric model over the marginal  $p_{\theta}(x) = \int p_{\theta}(x|z)p_{\theta}(z)dz$ . However, since the marginal is intractable a variational approximation  $q_{\phi}(z|x) \approx p_{\theta}(z|x)$  is proposed instead. The log probability  $log(p_{\theta}(x))$  is then developed in to the tractable VAE loss comprised of the Evidence Lower Bound (ELBO) and KL regularization terms:  $\mathcal{L}_{RO} = \mathcal{L}_{RO}$ 

 $\mathbb{E}_{q_{\phi}(z|x)}\left[\log\left(p_{\theta}(x|z)\right)\right] - D_{KL}\left(q_{\phi}(z|x) \bigg| \bigg| p_{\theta}(z)\right). \ q_{\phi}(z|x)$ is modeled using a stochastic neural encoder having it's final activation used as parameters for the assumed variational distribution (typically a spherical gaussian with parameters  $\mu, \Sigma$ ). Each forward pass emulates a stochastic realization  $z \in Z$  from these parameters by using the 'reparameterization trick':  $z = \mu + \epsilon \cdot \Sigma$  for some unparameterized scalar  $\epsilon \sim N(0,1)$  s.t. a backwards pass is possible. Higgins et al. (2017) later proposed the  $\beta$ -autoencoder introducing a hyper parameter  $\beta$  over the KL term to control the regularization-reconstruction tradeoff. Alemi et al. (2017) introduced the Variational Information Bottleneck (VIB) as a variational approximation for an upper bound to the IB objective for classifier DNN optimization: Upper bounds for I(Z,Y), I(X,Z) are derived from the identity  $D_{KL}\left( ext{True probability} \middle| \middle| ext{Variational approximation} \right) \, \geq \, 0$ and used to form an upper bound for the IB functional. This upper bound is approximated using variational approximations for  $p^*(y|z), p^*(z)$  similarly to VAEs. This approximation to an upper bound over the IB objective is empirically estimated as Cross entropy and a beta scaled KL regularization term as in  $\beta$ -autoencoders and is optimized over the training data S using Monte Carlo sampling and the reparameterization trick. VIB was evaluated over MNIST and ImageNet and, while causing a slight reduction in test-accuracy, it generated substantial improvements in robustness to adversarial attacks. Alemi et al. (2018) found that as the ELBO loss in VAEs depends solely on image reconstruction it does not necessarily induce a better quality modeling of the marginal  $p_{\theta}(z)$ , hence not necessarily a better representation learned. This gap is attributed to powerful decoders being overfitted. It is suggested to keep  $\beta$  values under 1 and monitor the rate-distortion tradeoff as well as cross-entropy loss.

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Additional noteworthy contributions to this field have been made in recent years by Achille & Soatto (2018); Wieczorek & Roth (2019); Fischer (2020) and others. However, a detailed review of these works is beyond the scope of this paper.

### 2.4. Non IB information theoretic regularization

Label smoothing (Szegedy et al., 2016) and entropy regularization (Pereyra et al., 2017) both regularize classifier DNNs by increasing the entropy of their output. This is done either directly with an entropy term in the loss function,  $\beta \cdot H\left(p_{\theta}(y|x)\right)$ , or by smoothing the training data labels. Applying both methods was demonstrated to improve test accuracy and model calibration. In the current work a similar conditional entropy term emerges from the derivation of the new upper bound for the IB objective as shown in Section 3.

# 3. From VIB to VUB

The VIB loss (Alemi et al., 2017) consists of a Cross-Entropy (CE) term and a KL regularization term, similar to the VAE loss. The KL term is derived from a bound on the IB rate term I(X;Z), while the CE term from a bound on the IB distortion term I(Z;Y) = H(Y) - H(Y|Z). When deriving the distortion term the entropy term H(Y) is ignored as it is constant and does not effect optimization, while the conditional entropy term H(Y|Z) is derived into a cross entropy term. We note that since Y is unknown any optimization on Z, including CE, depends on our decoder model of Y. Following this logic we reintroduce the omitted H(Y) term into the objective. We replace the unknown H(Y) with a variational approximation of the decoder's entropy, which provides a lower bound.

#### 3.1. IB upper bound

We begin by establishing a new upper bound for the IB functional, starting with the same derivation as shown in VIB.

We begin by bounding I(Z; X):

$$I(Z;X) = \int \int p^*(x,z)log(p^*(z|x)) dxdz$$
$$-\int p^*(z)log(p^*(z)) dz$$
(1)

For any probability distribution r we have that  $D_{KL}(p^*(z), r(z)) \ge 0$ , it follows that:

$$\int p^*(z)log\left(p^*(z)\right)dz \ge \int p^*(z)log\left(r(z)\right)dz \quad (2)$$

And so:

$$I(Z;X) \stackrel{2}{\leq} \int \int p^*(x)p^*(z|x)log\left(\frac{p^*(z|x)}{r(z)}\right)dxdz$$
 (3)

We proceed by bounding I(Z; Y):

For any probability distribution c we have that  $D_{KL}\left(p^*(y|z),c(y|z)\right)\geq 0$ , it follows that:

$$\int p^*(y|z)\log\left(p^*(y|z)\right)dy \ge \int p^*(y|z)\log\left(c(y|z)\right)dy$$
(4)

And so:

$$\begin{split} I(Z;Y) &= \int \int p^*(y,z)log\left(\frac{p^*(y,z)}{p^*(y)p^*(z)}\right)dydz\\ &\stackrel{4}{\geq} \int \int p^*(y|z)p^*(z)log\left(\frac{c(y|z)}{p^*(y)}\right)dydz\\ &= \int \int p^*(y,z)log\left(c(y|z)\right)dydz + H_{p^*}(Y) \end{split} \tag{5}$$

We continue bounding I(Z;Y) without discarding the entropy of Y:

$$\geq \int \int p^*(y,z)log\left(c(y|z)\right)dydz \\ +min\left\{H_{p^*}(Y),H_c(Y|Z)\right\} \tag{6}$$

We further develop this term using the markov chain  $Z \leftarrow X \leftarrow Y$  and total probability:

$$I(Z;Y) \ge \int \int \int p^*(x)p^*(y|x)p^*(z|x)\log(c(y|z)) dxdydz$$

$$-\min\left\{H_{p^*}(Y), -\int \int c(y,z)\log(c(y|z)) dydz\right\}$$
(7)

We define  $L_{UB}$ : A new upper bound for the IB functional.  $L_{UB}$  is composed of the new bound on the distortion term derived in Equation 7 together with the previously bound on the rate term derived in Equation 3:

$$L_{UB} \equiv \int \int p^*(x)p^*(z|x)log\left(\frac{p^*(z|x)}{r(z)}\right)dxdz$$
$$-\int \int \int p^*(x)p^*(y|x)p^*(z|x)log\left(c(y|z)\right)dxdydz$$
$$+min\left\{H_{p^*}(Y), -\int \int c(y,z)log\left(c(y|z)\right)dydz\right\} (8)$$

It is easy to verify that the derivation holds for all  $\beta \geq 0$  such that  $L_{IB} = \beta \cdot I(Z; X) - I(Z; Y)$ .

#### 3.2. Variational approximation

We follow the same variational approach as in VIB. We define  $L_{VUB}$  as a new tractable upper bound for the IB functional. Let  $p^*(x, y, z)$  be the unknown joint distribution, e(z|x) a variational encoder approximating  $p^*(z|x)$ ,

c(y|z) a variational classifier approximating  $p^*(y|z)$ . We reintroduce  $\beta$  to allow tuning of the KL term and replace the intractable  $p^*(z)$  is with the variational approximation r(z).

$$L_{VUB} \equiv \beta \int \int p^{*}(x)e_{\phi}(z|x)log\left(\frac{e_{\phi}(z|x)}{r(z)}\right)dxdz$$

$$-\int \int \int p^{*}(x)p^{*}(y|x)e_{\phi}(z|x)log\left(c_{\lambda}(y|z)\right)dxdydz$$

$$-min\left\{H_{p^{*}}(Y),\right.$$

$$-\int \int \int p^{*}(x)e_{\phi}(z|x)c_{\lambda}(y|z)log\left(c_{\lambda}(y|z)\right)dxdydz\right\}$$

$$\geq L_{IB}$$

# 3.3. Empirical estimation

We proceed to model VUB using DNNs and optimize it using Monte Carlo sampling over the training data  $\mathcal{D}$ . Let  $e_{\phi}$  be a stochastic DNN encoder with parameters  $\phi$  applying the reparameterization trick such that  $e_{\phi}(x) \sim N(\mu, \Sigma)$ . Let  $C_{\lambda}$  be a discrete classifier DNN parameterized by  $\lambda$  such that  $C_{\lambda}(\hat{z}) \sim Categorical$ .

$$\hat{L}_{VUB} \equiv \frac{1}{N} \sum_{n=1}^{N} \left[ \beta \cdot D_{KL} \left( e_{\phi}(x_n) \middle| r(z) \right) - P^*(y_n) \cdot \log \left( C_{\lambda} \left( e_{\phi}(x_n) \right) \right) - \min \left\{ H(\hat{Y}), H\left( C_{\lambda} \left( e_{\phi}(x_n) \right) \right) \right\} \right]$$

$$(10)$$

As in VIB and VAE  $e_{\phi}(x)$  is a computed as spherical gaussian by using the first half of the encoder's output entries as  $\mu$  and the second as the diagonal  $\Sigma$ .

#### 3.4. Interpretation

VUB is in fact VIB regulated by a conditional entropy term -H(Y|Z) similarly to the confidence penalty suggested by Pereyra et al. (2017). Hence, VUB adds regularization over the classifier preventing it to overfit the embeddings. This is a possible remedy to the discrepancies in the ELBO loss observed by Alemi et al. (2018).

In terms of tightness we have that VUB is a tighter theoretical bound on IB than VIB for any Y s.t. H(Y) > 0, and a tighter empirical bound for all Y.

# 4. Experiments

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We follow the experimental setup proposed by Alemi et al. (2017), extending it to NLP tasks as well. Image classification models were trained on the first 500,000 samples of the ImageNet 2012 dataset (Deng et al., 2009) and text classification over the IMDB sentiment analysis dataset (Maas et al., 2011). For each dataset, a competitive pre-trained model (Vanilla model) was evaluated and then used to encode embeddings. These embeddings were then used as a dataset for a new stochastic classifier net with either a VIB or a VUB loss function. Stochastic classifiers consisted of two ReLU activated linear layers of the same dimensions as the pre-trained model's logits (2048 for image and 768 for text classification), followed by reparameterization and a final softmax activated FC layer. Learning rate was  $10^{-4}$  and decaying exponentially with a factor of 0.97 every two epochs. Batch sizes were 32 for ImageNet and 16 for IMDB. We used a single forward pass per sample for inference. Each model was trained and evaluated 5 times per  $\beta$  value with consistent performance. Beta values of  $\beta = 10^{-i}$  for  $i \in \{1, 2, 3\}$  were tested since previous studies indicated this is the best range for VIB (Alemi et al., 2017; 2018). Each model was evaluated using test set accuracy and robustness to various adversarial attacks over the test set. For image classification we employed the untargeted Fast Gradient Sign (FGS) attack (Goodfellow et al., 2015) as well as the targeted CW  $L_2$  optimization attack (Carlini & Wagner, 2017), (Kaiwen, 2018). For text classification we used the untargeted Deep Word Bug attack (Gao et al., 2018), (Morris et al., 2020) as well as the untargeted PWWS attack (Ren et al., 2019). All models were trained using an Nvidia RTX3080 GPU. Code to reconstruct the experiments is provided in the code & data appendix.

#### 4.1. Image classification

A pre-trained inceptionV3 (Szegedy et al., 2016) base model was used and achieved a 77.21% accuracy on the image-net 2012 validation set (Test set for image-net is unavailable). Note that inceptionV3 yields a slightly worse single shot accuracy than inceptionV2 (80.4%) when run in a single model and single crop setting, however we've used InceptionV3 over V2 for simplicity. Each model was trained for 100 epochs.

## 4.1.1. EVALUATION AND ANALYSIS

Image classification evaluation results are shown in Table 1, examples of successful attacks are shown in Figures 5, 4. The empirical results presented in Table 1 confirm that while VIB reduces performance on the validation set, it substantially improves robustness to adversarial attacks. Moreover, these results demonstrate that VUB significantly outperforms VIB in terms of validation accuracy while providing

| β             | Val ↑                 | $\mathop{\bf FGS}_{\epsilon=0.1}\downarrow$ | $FGS_{\epsilon=0.5} \downarrow$ | CW↑              |  |
|---------------|-----------------------|---------------------------------------------|---------------------------------|------------------|--|
| Vanilla model |                       |                                             |                                 |                  |  |
| -             | 77.2%                 | 68.9%                                       | 67.7%                           | 788              |  |
| VIB models    |                       |                                             |                                 |                  |  |
| $10^{-3}$     | <b>73.7%</b> ±.1%     | <b>59.5%</b> ±.2%                           | <b>63.9%</b><br>±.2%            | <b>3917</b> ±291 |  |
| $10^{-2}$     | <b>72.8%</b><br>±.1%  | <b>53.5%</b> ±.2%                           | <b>62.0%</b><br>±.1%            | <b>3318</b> ±293 |  |
| $10^{-1}$     | <b>72.1%</b><br>±.01% | <b>58.4%</b> ±.1%                           | <b>62.0%</b><br>±.1%            | <b>3318</b> ±293 |  |
| VUB models    |                       |                                             |                                 |                  |  |
| $10^{-3}$     | <b>75.5%</b> ±.03%    | <b>62.8%</b><br>±.1%                        | <b>66.4%</b><br>±.1%            | <b>2666</b> ±140 |  |
| $10^{-2}$     | <b>75.0%</b> ±.05%    | <b>57.6%</b> ±.2%                           | <b>64.3%</b><br>±.1%            | 1564<br>±218     |  |
| $10^{-1}$     | <b>74.8%</b> ±0.09%   | <b>57.9%</b> ±.5%                           | <b>64.8%</b> ±.5%               | 3575<br>±456     |  |

Table 1. Image-net evaluation scores for vanilla, VIB and VUB models, average over 5 runs with standard deviation. First column is performance on the image-net validation set (higher is better  $\uparrow$ ). Second and third columns are the % of successful FGS attacks at  $\epsilon=0.1,0.5$  (lower is better  $\downarrow$ ). Fourth column is the average  $L_2$  distance for a successful Carlini Wagner  $L_2$  targeted attack (higher is better  $\uparrow$ ).

competitive robustness to attacks similarly to VIB. A comparison of the best VIB and VUB models further substantiates these findings, with statistical significance confirmed by a p-value of less than 0.05 in a Wilcoxon rank sum test.

In addition to the evaluation metrics, we measured approximated rate and distortion throughout training and plotted them on the information curve as shown in Figure 3. We notice recurring patterns of distortion reduction followed by rate increase, resembling the ERM and representation compression stages described by Shwartz-Ziv & Tishby (2017).

#### 4.2. Text classification

A fine tuned BERT uncased (Devlin et al., 2019) base model was used and achieved a 95.5% accuracy on the IMDB sentiment analysis test set. Each model was trained for 150 epochs and the first 200 entries in the test set used for evaluation and adversarial attacks.

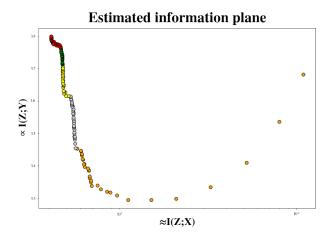


Figure 3. Estimated information plane metrics per epoch for VUB trained on IMDB with  $\beta=0.001$ . I(Z;X) is approximated by H(R)-H(Z|X) and  $\frac{1}{CE(Y;\hat{Y})}$  is used as an analog for I(Z;Y). The epochs have been grouped and color-coded in intervals of 30 epochs in the order: Orange (0-30), gray (30-60), yellow (60-90), green (90-120) and red (120-150). We notice recurring patterns of distortion reduction followed by rate increase, resembling the ERM and representation compression stages described by Shwartz-Ziv & Tishby (2017).

#### Targeted CW attacks for VIB $\beta$ =0.01



Targeted CW attacks for VUB  $\beta$ =0.01





Figure 4. Successful targeted CW attack examples. Images are perturbations of previously successfully classified instances from the ImageNet validation set. The target label is 'Soccer ball'. Average  $L_2$  distance required for a successful attack is shown on the left. The higher the required  $L_2$  distance the greater the visible change required to fool the model. Original and wrongly assigned labels are listed at the top of each image. Mind the difference in noticeable change as compared to FGS perturbations and between VIB and VUB perturbations.

| β                    | Test↑        | DWB↓        | PWWS↓        |
|----------------------|--------------|-------------|--------------|
|                      | Vanilla mode | l           |              |
| -                    | 95.5%        | 75.9%       | 100%         |
|                      | VIB models   |             |              |
| $10^{-3}$            | 91.0%        | 35.1%       | 41.6%        |
|                      | $\pm 1.0\%$  | $\pm 4.4\%$ | $\pm 6.6\%$  |
| $10^{-2}$            | 90.8%        | 41.0%       | 62.9%        |
|                      | $\pm 0.5\%$  | $\pm 4.8\%$ | $\pm 14.3\%$ |
| $\overline{10^{-1}}$ | 89.4%        | 90.0%       | 99.1%        |
|                      | $\pm .9\%$   | $\pm 8.0\%$ | $\pm 0.9\%$  |
|                      | VUB models   |             |              |
| $\overline{10^{-3}}$ | 93.2%        | 27.5%       | 28.4%        |
|                      | $\pm .5\%$   | $\pm 2.0\%$ | $\pm 1.3\%$  |
| $10^{-2}$            | 92.6%        | 30.8%       | 50.0%        |
|                      | $\pm .8\%$   | $\pm 2.0\%$ | $\pm 4.8\%$  |
| $10^{-1}$            | 89.2%        | 99.2%       | 100%         |
|                      | $\pm 2.0\%$  | $\pm 0.5\%$ | $\pm 0\%$    |

Table 2. Evaluation for vanilla, VIB and VUB models, average over 5 runs with standard deviation over the IMDB dataset. First column is performance on the test set (higher is better ↑), second is % of successful Deep Word Bug attacks (lower is better ↓), third column is % of successful PWWS attacks (lower is better ↓).

#### 4.2.1. EVALUATION AND ANALYSIS

Text classification evaluation results are shown in Table 2, examples of successful attacks are shown in Figure 3. In this modality VUB significantly outperforms VIB in both test set accuracy and robustness to both attacks. A comparison of the best VIB and VUB models further substantiates these findings, with statistical significance confirmed by a p-value of less than 0.05 in a Wilcoxon rank sum test.

#### 5. Discussion

Our study strengthens the argument for using the Information Bottleneck combined with variational approximations to obtain robust models that can withstand adversarial attacks. By deriving a tighter bound on the IB functional, we demonstrate it's utility as the Variational Upper Bound (VUB) objective for neural networks. We demonstrate that VUB outperforms the Variational Information Bottleneck (VIB) in terms of test accuracy while providing similar or superior robustness to adversarial attacks in challenging classification tasks of different modalities.

Comparing VIB and VUB we observe that both methods promote a disentangled latent space by using a stochastic factorized prior, as suggested by Chen et al. (2018). In

# Text perturbed with DWB

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gnreat historical movie, will not allow a viewer to leave once you begin to watch. View is presented differently than displayed by most school books on this sSubject [...]

#### **Text perturbed with PWWS**

the acting, costumes, music, cinematography and sound are all astounding dumbfounding given the production 's austere locales.

Table 3. Examples of a successful DWB an PWWS attacks on a vanilla Bert model fine tuned over the IMDB dataset. The original labels were 'Positive sentiment'. Perturbations including inserted tokens marked in boldface and removed tokens marked in strikethrough, change the classification to 'Negative sentiment'.

addition, both methods utilize KL regularization, enforcing clustering around a 0 mean which might increase latent smoothness. These traits can make it difficult for minor perturbations to significantly alter latent semantics, making the models more robust to attacks. In the case of VUB, the enhanced results induced by classifier regularization not only reinforce previous studies on the ELBO function, which suggest that overly powerful decoders diminish the quality learned representations (Alemi et al., 2018), but also align with the confidence penalty proposed by Pereyra et al. (2017).

We also observed that in many cases VIB achieves lower validation set Cross-Entropy while VUB achieves significantly higher test set accuracy. We attribute this gap to the VUB models becoming more calibrated, and we suggest that practitioners also monitor validation set accuracy and rate distortion ratio and during training. These metrics may be more informative indicators of model performance than validation set Cross-Entropy alone, as validation Cross-Entropy could increase as models become more calibrated.

We made another interesting observation during our study regarding information plane behavior throughout the training process. While previous research has documented the occurrence of error minimization and representation compression phases, our work revealed that these phases can occur in cycles throughout training. This finding is particularly noteworthy because previous studies observed this phenomenon in simple toy problems, whereas our research demonstrated it in a complex task with an unknown distribution and high dimensionality. This suggests that the behavior of the information plane is not limited to simplified scenarios but is a characteristic of the learning process in more challenging tasks as well.

In conclusion, while the IB and its variational approximations do not provide a complete theoretical framework for

DNN data modeling and regularization, they offer a strong, measurable, and theoretically-grounded approach. VUB is presented as a tractable and tighter upper bound of the IB functional that can be easily adapted to any classifier DNN, including transformer based text classifiers, to significantly increase robustness to various adversarial attacks while inflicting minimal decrease in performance. This study opens many opportunities for further research. Besides further improvements to the upper bound, it is intriguing to use VUB in self-supervised learning and in generative tasks. Other possible directions, including measuring model calibration as proposed by Achille & Soatto (2018) are left for future work.

# Untargeted FGS attacks for VIB $\beta$ =0.01



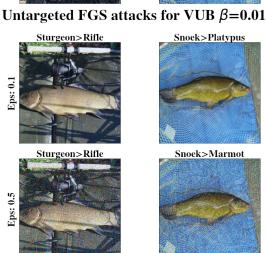


Figure 5. Successful untargeted FGS attack examples. Images are perturbations of previously successfully classified instances from the ImageNet validation set. Perturbation magnitude is determined by the parameter  $\epsilon$  shown on the left, the higher the more perturbed. Notice the deterioration of image quality as  $\epsilon$  increases. Original and wrongly assigned labels are listed at the top of each image.

#### References

- Achille, A. and Soatto, S. Information dropout: Learning optimal representations through noisy computation. *IEEE Trans. Pattern Anal. Mach. Intell.*, 40(12):2897–2905, 2018. URL http://dblp.uni-trier.de/db/journals/pami/pami40.html#AchilleS18.
- Alemi, A. A., Fischer, I., Dillon, J. V., and Murphy, K. Deep variational information bottleneck. In *Proceedings of the International Conference on Learning Representations (ICLR)*, Google Research, 2017.
- Alemi, A. A., Poole, B., Fischer, I., Dillon, J. V., Saurous, R. A., and Murphy, K. Fixing a broken elbo. In *Proceedings of Machine Learning Research*, volume 80, pp. 159–168, PMLR, 2018. URL http://dblp.uni-trier.de/db/conf/icml/icml2018.html#AlemiPFDS018.
- Amjad, R. A. and Geiger, B. C. Learning representations for neural network-based classification using the information bottleneck principle. *IEEE Trans. Pattern Anal. Mach. Intell.*, 42(9):2225–2239, 2020. URL http://dblp.uni-trier.de/db/journals/pami/pami42.html#AmjadG20.
- Blahut, R. E. Computation of channel capacity and rate distortion function. *IEEE Transactions on Information Theory*, IT-18:460–473, 1972. doi: https://ieeexplore.ieee.org/document/1054855. URL https://ieeexplore.ieee.org/document/1054855.
- Carlini, N. and Wagner, D. A. Towards evaluating the robustness of neural networks. In *IEEE Symposium on Security and Privacy*, pp. 39–57. IEEE Computer Society, 2017. URL http://dblp.uni-trier.de/db/conf/sp/sp2017.html#Carlini017.
- Chechik, G. et al. Gaussian information bottleneck.

  In Advances in Neural Information Processing

  Systems, 2003. URL https://proceedings.
  neurips.cc/paper/2003/hash/
  7e05d6f828574fbc975a896b25bb011e-Abstract.
  html.
- Chen, T. Q., Li, X., Grosse, R. B., and Duvenaud, D. Isolating sources of disentanglement in variational autoencoders. In *Proceedings of the 32nd International Conference on Neural Information Processing Systems*, pp. 2615–2625, 2018. URL http://dblp.uni-trier.de/db/conf/nips/nips2018.html#ChenLGD18.
- Deng, J., Dong, W., Socher, R., Li, L.-J., Li, K., and Fei-Fei, L. Imagenet: A large-scale hierarchical image database.

- In 2009 IEEE conference on computer vision and pattern recognition, pp. 248–255. Ieee, 2009.
- Devlin, J., Chang, M.-W., Lee, K., and Toutanova, K. Bert: Pre-training of deep bidirectional transformers for language understanding. In *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers)*, pp. 4171–4186, Minneapolis, Minnesota, 2019. URL https://www.aclweb.org/anthology/N19-1423.
- Fischer, I. The conditional entropy bottleneck. Entropy, 22(9):999, 2020. URL http://dblp.uni-trier.de/db/journals/ entropy/entropy22.html#Fischer20.
- Gao, J., Lanchantin, J., Soffa, M. L., and Qi, Y. Black-box generation of adversarial text sequences to evade deep learning classifiers. In 2018 IEEE Security and Privacy Workshops (SPW), pp. 50–56. IEEE, 2018.
- Goodfellow, I. J., Shlens, J., and Szegedy, C. Explaining and harnessing adversarial examples. In *ICLR* (*Poster*), 2015. URL http://dblp.uni-trier.de/db/conf/iclr/iclr2015.html#GoodfellowSS14.
- Guo, C., Pleiss, G., Sun, Y., and Weinberger, K. Q. On calibration of modern neural networks. In *International conference on machine learning*, pp. 1321–1330. PMLR, 2017.
- Higgins, I., Matthey, L., Pal, A., Burgess, C., Glorot, X., Botvinick, M., Mohamed, S., and Lerchner, A. betavae: Learning basic visual concepts with a constrained variational framework. In *ICLR (Poster)*, 2017.
- Kaiwen. pytorch-cw2, 2018. URL https://github.com/kkew3/pytorch-cw2. GitHub repository.
- Kingma, D. P. and Welling, M. Auto-encoding variational bayes. In 2nd International Conference on Learning Representations, ICLR 2014, Banff, AB, Canada, April 14-16, 2014, Conference Track Proceedings, 2014.
- Kingma, D. P. and Welling, M. An introduction to variational autoencoders. *Foundations and Trends in Machine Learning*, 12(4):307–392, 2019. URL http://dblp.uni-trier.de/db/journals/ftml/ftml12.html#KingmaW19.
- Maas, A., Daly, R. E., Pham, P. T., Huang, D., Ng, A. Y., and Potts, C. Learning word vectors for sentiment analysis. In *Proceedings of the 49th annual meeting of the association for computational linguistics: Human language technologies*, pp. 142–150, 2011.

Morris, J., Lifland, E., Yoo, J. Y., Grigsby, J., Jin, D., and Qi,
 Y. Textattack: A framework for adversarial attacks, data augmentation, and adversarial training in nlp. In *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing: System Demonstrations*,
 pp. 119–126, 2020.

- Painsky, A. and Tishby, N. Gaussian lower bound for the information bottleneck limit. *J. Mach. Learn. Res.*, 18:213:1–213:29, 2017. URL http://dblp.uni-trier.de/db/journals/jmlr/jmlr18.html#PainskyT17.
- Pereyra, G., Tucker, G., Chorowski, J., Kaiser, L., and Hinton, G. E. Regularizing neural networks by penalizing confident output distributions. In *Proceedings of the International Conference on Learning Representations*, OpenReview.net, 2017. URL http://dblp.uni-trier.de/db/conf/iclr/iclr2017w.html#PereyraTCKH17.
- Ren, S., Deng, Y., He, K., and Che, W. Generating natural language adversarial examples through probability weighted word saliency. In *Proceedings of the 57th annual meeting of the association for computational linguistics*, pp. 1085–1097, 2019.
- Shwartz-Ziv, R. and Tishby, N. Opening the black box of deep neural networks via information, 2017. URL http://arxiv.org/abs/1703.00810. 19 pages, 8 figures.
- Slonim, N. *The information bottleneck: Theory and applications*. PhD thesis, Hebrew University of Jerusalem Jerusalem, Israel, 2002.
- Szegedy, C., Vanhoucke, V., Ioffe, S., Shlens, J., and Wojna, Z. Rethinking the inception architecture for computer vision. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 2818–2826, 2016.
- Tishby, N. and Zaslavsky, N. Deep learning and the information bottleneck principle, 2015.
- Tishby, N., Pereira, F. C., and Bialek, W. The information bottleneck method. In *The 37th annual Allerton Conference on Communication, Control, and Computing.*, Hebrew University, Jerusalem 91904, Israel, 1999.
- Wieczorek, A. and Roth, V. On the difference between the information bottleneck and the deep information bottleneck. *CoRR*, abs/1912.13480, 2019. URL http://dblp.uni-trier.de/db/journals/corr/corr1912.html#abs-1912-13480.
- Ying, X. An overview of overfitting and its solutions. *Journal of Physics: Conference Series*, 1168 (2):022022, feb 2019. doi: 10.1088/1742-6596/1168/2/

022022. URL https://dx.doi.org/10.1088/1742-6596/1168/2/022022.