On Variational Generalization Bounds for Unsupervised Visual Recognition

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Abstract

Recent advancements in generalization bounds have led to the development of tight information theoretic and data-dependent measures. Although generalization bounds reduce bias in estimates, they often suffer from tractability during empirical evaluation. The lack of a uniform criterion for estimation of Mutual Information (MI) and selection of divergence measures in conventional bounds hinders utility to sparse distributions. To that end, we revisit generalization through the lens of variational bounds. We identify hindrances based on bias, variance and learning dynamics which prevent accurate approximations of data distributions. Our empirical evaluation carried out on large-scale unsupervised visual recognition tasks highlights the necessity for variational bounds as generalization objectives for learning complex data distributions. Approximated estimates demonstrate low variance and improved convergence in comparison to conventional generalization bounds. Lastly, based on observed hindrances, we propose a theoretical alternative which aims to improve learning and tightness of variational generalization bounds. The proposed approach is motivated by contraction theory and yields a lower bound on MI.

1 Introduction

Generalization bounds provide tight measures which facilitate the learning of distributions under sparse data. The work of Russo et. al. [1] has led to drastic improvements [2, 3] in bounding generalization error with information theoretic metrics. The surge of information theoretic metrics [2, 4] has further motivated improvements in bias reduction for control measurements [**?**]. While generalization bounds tighten the dynamics of sparse learning, a tighter approximation often hurts the performance in the presence of out-of distribution samples [5]. In many such scenarios, it is difficult to empirically evaluate the performance of the bound [6]. Additionally, the abundance of divergence metrics does not provide a selection criterion for an optimal information theoretic entity [7, 8]. This allows one to rethink the feasibility of conventional bounds in practical scenarios.

Variational bounds [9] are a class of probabilistic bounds which depict increasing potential for learning [5, 10, 11]. A typical variational bound utilizes a tractable data distribution which can be approximated with limited data samples. This property of variational measures motivates data-efficient learning [12]. Tractibility of variational bounds for information maximization and minimization allows multiple objective functions to be realisable in a given problem setting [9]. Variational bounds can then be flexibly modeled as lower and upper bounding measures of information [9]. However, large-scale utilization of multi-sample variational bounds is an open problem for unsupervised learning tasks [9]. Data-efficient learning in conjunction with tractable compatibility to data distributions presents variational bounds as suitable candidates for learning objective functions.

We revisit the regime of generalization bounds from the perspective of information theoretic and variational distributions. The work highlights the suitability of variational bounds in comparison to

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conventional generalization bounds which emphasize only on the bias in data estimates. Variational objectives tackle high bias as well as high variance estimates. Our main contributions are threefold-

- We revisit generalization in light of variational learning and identify hindrances which prevent accurate approximations of data distributions.
- We empirically demonstrate the suitability of variational generalization bounds on unsupervised visual recognition tasks wherein the data distribution is inherently challenging to approximate. Our evaluation highlights the necessity for variational generalization bounds.
- We conjecture a theoretical alternative which aims to address the hindrances discovered in learning variational generalization bounds. The proposed approach is motivated by contraction theory and yields a lower bound on MI.

2 Related Work

Variational Bounds: A number of methods [9, 5, 13, 11, 12] introduce variational bounds for information-based learning. MINE [5] presents the estimation of MI utilizing gradient descent for high-dimensional random variables. Suitability of MINE leads to improved adversarial generative models and supervised classification tasks. InfoMAX [13], extends the MI framework by simultaneously estimating and maximizing information between output representations and input prior distributions. InfoMAX scales well to unsupervised learning scenarios and sparse latent distributions. While, MINE and InfoMAX highlight the practical utility of information estimation, they do so at the cost of large data requirements from the input distribution. CPC [11] and CPCv2 [12] aid data-efficient learning by introducing the InfoNCE bound. The InfoNCE objective eliminates the need for explicit estimation of MI by providing a lower bound on MI. InfoNCE being a multi-sample bound [9], scales well in the number of data samples in-distribution. However, the objective is hindered by large batch sizes and is not tight for large values of MI. The recently proposed interpolation bounds [9] extend the InfoNCE setup towards a continuum of bounds which trade-off bias with variance. Additionally, the bound is tight for varying batch sizes. Our work is orthogonal to the proposed interpolation scheme and extends it to the generalization setup.

Generalization Bounds: The pivotal work of [1] provides a lower-bound on MI based on information-theoretic measures [14, 7]. The MI bound [15] is further improved as a result of tight lower bounds on MI minimizing the generalization error [2, 4]. Additional measures such as data-dependent estimates [3] and the specific choice of distributions [16] extend the application of lower bounds to stochastic learning dynamics [4, 17] and differential privacy [1**?**]. The bounds are further sharpened using conditional MI [18] in a sample-based framework [19] which extends the data-dependent scheme of [3]. A more suitable application is the setting of adaptive control [6] which is based on high stochasticity stemming from continuous measurements. The bound provided in [6] aims to address this problem with the introduction of $alpha$ divergence metrics [8] which serve as a lower bound on MI. While the bound is proven to be theoretically tight, its application and empirical evaluation remain an open problem in literature. We aim to leverage the theoretical contributions of [6] in order to provide a variational alternative which can be empirically realised.

Unsupervised Visual Recognition: One of the main applications of information-theoretic bounds is unsupervised learning for visual recognition tasks [10]. The information maximization framework [13] reduces local sparsity and motivates the learning of richer representations [11]. Multi-sample bounds such as InfoNCE in CPC [11] and CPCv2 [12] contrast augmented representations with actual input samples in order to maximize MI among local pixels. MOCO [20, 21] extends the setup of InfoNCE further with the pretext contrast as a dictionary-lookup task. InfoNCE bound is combined with a momentum encoder which maximizes MI as a slow moving average of input and augmented samples. SimCLR [22] builds on the MOCO framework by maximizing the internal agreement between representations. While unsupervised representation learning methods adopt lower bounds on MI, they do so at the cost of large batch sizes. Since the InfoNCE bound is lose at small batch sizes, large architectures lean towards pretraining alternatives [23] rather than improving lower bounds. The work of [10] adapts InfoNCE bound based on parameteric and non-parameteric learning of visual instance discrimination. The multi-sample classification is casted to a binary discrimination setup, hence providing improved generalization and consistent performance. Based on this insight, we adopt the instance discrimination setup of [10] for our experiments.

3 Preliminaries

We review the information-theoretic setup for generalization and variational bounds. Let X and Y be a pair of random variables denoting the input and output data distributions $p(x)$ and $p(y)$ respectively. The mutual information $I(X;Y)$ between X and Y is a reparameterization-invariant measure of dependency consisting of the joint distribution $p(x,y)$and can be mathematically expressed as follows,

$$I(X;Y) = \mathbb{E}_{p(x,y)}[\log \frac{p(x|y)}{p(x)}] = \mathbb{E}_{p(x,y)}[\log \frac{p(y|x)}{p(y)}] \tag{1}$$

Equation 1 can be further simplified by exapnding the expectation,

$$I(X;Y) = \sum_{y} p(x|y)p(y) \log \frac{p(x|y)}{p(x)} = \mathbb{E}_{p(y)}[D_{KL}(p(x|y)||p(x))] \tag{2}$$

D_{KL} in Equation 2 denotes the Kullback-Liebler (KL) Divergence [24] which is a divergence metric. D_{KL} belongs to the general class of $\phi-$divergence metrics $D_{\phi}(P(x)||Q(y))$ which quantify the similarity between any two data distributions $P(x)$ and $Q(y)$. The general form of a ϕ-divergence, with ϕ being a convex and lower semi-continuous function such that $\phi(1) = 0$, is expressed in Equation 3. Utilizing $\phi(t) = t \log t$ in Equation 3 yields $D_{\phi}(P(x)||Q(y)) = D_{KL}(P(x)||Q(y))$.

$$D_{\phi}(P(x)||Q(y)) = \sum_{y} Q(y)\phi(\frac{P(x)}{Q(y)}) \tag{3}$$

Generalization bounds make use of random variables with a cumulant-generation [25] function $\psi(\lambda) = \log \mathbb{E}[e^{\lambda x}]$ such that $\lambda \geq 0$. A random variable is called σ-sub-Gaussian if the argument of the log cumulant-generation function satisfies $\mathbb{E}[e^{\lambda x}] \leq e^{\frac{\lambda^2}{\sigma}^2}2$ for all $\lambda \in \mathbb{R}$ with σ^2 as the variance proxy or variance factor of the distribution.

4 When Do Bounds Hurt Learning?

The work of [9] throws light on the behavior of tractable distributions with high dimensional random variables. Based on the empirical characteristics of these bounds, one can identify the hindrances faced in generalization of the leanring algorithm (see Figure 1).

High Variance: Normalized upper and lower bounds aid in tractability of variational distributions when the data to be learned is long-tailed. However, these bounds demonstrate high variance as a result of large MI estimates. A suitable alternative to normalized bounds is to adopt the framework of structured bounds. These bounds leverage the structure of the problem and yield a known conditional distribution $p(y|x)$ which is tractable as per the problem setting. Structured bounds are conveniently applicable to representation learning [11, 9] but do not necessarily scale to high-dimensional scenarios. Another alternative which provisions a conitional tractable distribution are reparameterization bounds. These bounds make use of an additional functional, known as the *critic*, which converts lower bounds on MI into upper bounds on KL divergence. The critic functional need not explicitly learn the mapping between x and y. However, reparameterization is only made feasible if the conditional distribution $p(y|x)$ is tractable.

High Bias: Unnormalized upper and lower bounds demonstrate high bias and hurt tractability of complex distributions. Primary reasons for instability in bounds is lack of a partition functional which normalizes MI estimates. [9] argues that requirement of a partition function presents high bias as a result of exponential distributions which may not be tractable. However, the work does not provide empirical evidence on their tractability which leaves the suitability of a normalization constant an pen question. A suitable alternative to address biased estimates is the adoption of density ratios which train the critic functional using a divergence metric. The Jensen-Shanon Divergence (JSD) is one such scheme which yields a lower-biased estimate of optimal critic. While training critics is theoretically suitable, empirical evaluations [9] demonstrate unstable convergence of exponential gradients.

A Failure to Learn: Biased and noisy estimates are the key hindrances in learning tractable distributions. To that end, [9] aptly proposes a continuum of multi-sample interpolation bounds which trade-off bias with variance. A simpler form of critic when applied to non-linear interpolation in InfoNCE samples yields a continuum of lower bounds on MI. The new bound can be manually

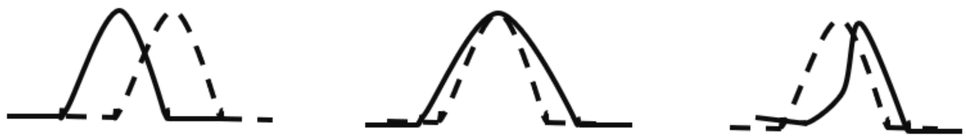

Figure 1: **Left** Conventional lose bounds suffer from high bias which hurts generalization of the learnt distribution, **Center** Learnt distribution is additionally hampered with noisy approximations, **Right** Biased estimates in conjunction with noisy dynamics hurt the completeness of learnt distribution.

tuned using γ which trades off bias with variance. Nonlinear interpolation bounds proposed in conjunction with MI saturate at $\log \frac{K}{\gamma}$ with K being the number of samples in the batch. Saturation of interpolation hurts the completeness of distribution and the bound fails to learn large MI estimates with inceasing batch sizes.

5 Variational Bounds for Generalization

This section provides insights into variational bounds as generelization measures of MI. Learning of variational bounds is discussed from the multi-sample and interpolation perspective. Nonlinear interpolation bounds give rise to the trade-off between bias and variance in estimates. Following generalization through this lens, we formulate an alternate approach with bias reduction as a contraction mapping. We extend our theoretical claims to previously discussed generalization bounds and discuss their formulations.

5.1 Learning Variational Bounds

InfoNCE: The InfoNCE objective is based on multi-sample unnormalized bounds. These bounds formulate multi-sample MI $I(X_1; Y)$ which is bounded by the optimal choice of critic $f(x, y)$. One such formulation is based on MINE [5] as presented in Equation 4.

$$I(X_1, Y) \geq 1 + \mathbb{E}_{p(x_{1:K})p(y|x_1)}[\log \frac{e^{f(x_1,y)}}{m(y; x_{1:K})}] - \mathbb{E}_{p(x_{1:K})p(y)}[\log \frac{e^{f(x_1,y)}}{m(y; x_{1:K})}] \tag{4}$$

Here $m(y; x_{1:K})$ is a Monte-Carlo estimate of the partition function $Z(y)$ and is mathematically expressed in Equation 5.

$$m(y; x_{1:K}) = \frac{1}{K}\sum_{k=1}^{K} e^{f(x_k,y)} \tag{5}$$

One can recover the InfoNCE bound (I_{NCE}) upon averaging over all K replicates in the last term of Equation 4 which yields 1. I_{NCE} can then be expressed as a lower bound on MI in Equation 6.

$$I(X; y) \geq \mathbb{E}[\frac{1}{K}\sum_{k=1}^{K} \log \frac{e^{f(x_i,y_i)}}{\frac{1}{K}\sum_{j=1}^{K} e^{f(x_k,y_j)}}] \triangleq I_{NCE} \tag{6}$$

Nonlinear Interpolation: The multi-sample framework of MINE can be further extended using a simpler formulation. A nonlinear interpolation between MINE and I_{NCE} bridges the gap between low-bias and high-variance estimates of MINE with high-bias and low-variance estimates of I_{NCE}. The nonlinear interpolation bound (I_{IN}) is expressed in Equation 7.

$$I_{IN} \triangleq 1 + \mathbb{E}_{p(x_{1:K})p(y|x_1)}[\log \frac{e^{f(x_1,y)}}{\gamma m(y; x_{1:K}) + (1-\gamma)q(y)}] - \mathbb{E}_{p(x_{1:K})p(y)}[\log \frac{e^{f(x_1,y)}}{\gamma m(y; x_{1:K}) + (1-\gamma)q(y)}] \tag{7}$$

While I_{NCE} is upper bounded by $\log K$, I_{IN} is upper bounded by $\log \frac{K}{\gamma}$. The control in bias-variance trade-off improves accuracy of estimates. However, the significance of γ remains an open question in the case of higher-order divergence metrics and large value of MI in practical settings.

ϕ-divergence:

5.2 Bias Reduction as Contraction

6 Experiments

6.1 Setup

6.2 Unsupervised Instant Discrimination

7 Conclusion

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