Reliable Estimation of KL Divergence using a Discriminator in Reproducing Kernel Hilbert Space

Sandesh Ghimire, Aria Masoomi, Jennifer Dy
Department of Electrical and Computer Engineering
Northeastern University
Boston, MA, USA
sandesh@ece.neu.edu, a.masoomi@northeastern.edu, jdy@ece.neu.edu

Abstract

Estimating Kullback–Leibler (KL) divergence from samples of two distributions is essential in many machine learning problems. Variational methods using neural network discriminator have been proposed to achieve this task in a scalable manner. However, we noted that most of these methods using neural network discriminators suffer from high fluctuations (variance) in estimates and instability in training. In this paper, we look at this issue from statistical learning theory and function space complexity perspective to understand why this happens and how to solve it. We argue that the cause of these pathologies is lack of control over the complexity of the neural network discriminator function and could be mitigated by controlling it. To achieve this objective, we 1) present a novel construction of the discriminator in the Reproducing Kernel Hilbert Space (RKHS), 2) theoretically relate the error probability bound of the KL estimates to the complexity of the discriminator in the RKHS space, 3) present a scalable way to control the complexity (RKHS norm) of the discriminator for a reliable estimation of KL divergence, and 4) prove the consistency of the proposed estimator. In three different applications of KL divergence – estimation of KL, estimation of mutual information and Variational Bayes – we show that by controlling the complexity as developed in the theory, we are able to reduce the variance of KL estimates and stabilize the training.

1 Introduction

Estimating Kullback–Leibler (KL) divergence from data samples is an essential component in many machine learning problems including Bayesian inference, calculation of mutual information or methods using information theoretic objectives. Variational formulation of Bayesian Inference requires KL divergence computation, which could be challenging when we only have finite samples from two distributions. Similarly, computation of information theoretic objectives like mutual information requires computation of KL divergence between the joint and the product of marginals.

KL divergence estimation from samples was studied thoroughly by Nguyen et al. [1] using a variational technique, convex optimization and RKHS norm regularization, while also providing theoretical guarantees and insights. However, their technique requires handling the whole dataset at once and is not scalable. Many modern models need to use KL divergence with large scale data, and often with neural networks, for example total correlation variational autoencoder (TC-VAE) [2], adversarial variational Bayes (AVB) [3], information maximizing GAN (InfoGAN) [4], and amortized MAP [5] all need to compute KL divergence in a deep learning setup. These large scale models have imposed new requirements on KL divergence estimation like scalability (able to handle large amount of data samples) and minibatch compatibility (compatible with minibatch-based optimization).
Methods like Nguyen et al. [1] are not suitable in the large scale setup. These modern needs were later met by modern neural network based methods such as variational divergence minimization (VDM) [6], mutual information neural estimation (MINE) [7], and discriminator based KL estimation with GAN-type objective [8,5]. A key attribute of these methods is that they are based on updating a neural-net based discriminator to estimate KL divergence from a subset of samples making them scalable and minibatch compatible. We, however, noticed that even in simple examples, these methods exhibited pathologies like unreliability (high fluctuation of estimates) or instability during training (KL estimates blowing up). Similar observations of instability of VDM and MINE have also been reported in the literature [8,9].

Why are these techniques unreliable? In this paper, we attempt to understand the core problem in the KL estimation using discriminator network. We look at it from the perspective of statistical learning theory and discriminator function space complexity and draw insights. Based on these insights, we propose that these fluctuations are a consequence of not controlling the smoothness and the complexity of the discriminator function space. Measuring and controlling the complexity of the function space itself becomes a difficult problem when the discriminator is a deep neural network. Note that naive approaches to bound complexity by the number of parameters would neither be guaranteed to yield meaningful bound [10], nor be easy to implement.

Therefore, we present the following contributions to resolve these challenges. First, we propose a novel construction of the discriminator function using deep network such that it lies in a smooth function space, the Reproducing Kernel Hilbert Space(RKHS). By utilizing the learning theory and the complexity analysis of the RKHS space, we bound the probability of the error of KL-divergence estimates in terms of the radius of RKHS ball and kernel complexity. Using this bound, we propose a scalable way to control the complexity by penalizing the RKHS norm. This additional regularization of the complexity is still linear, $O(m)$ in time complexity with the number of data samples. Then, we prove consistency of the proposed KL estimator using ideas from empirical process theory. Experimentally, we demonstrate that the proposed way of controlling complexity significantly improves KL divergence estimation and significantly reduce the variance. In mutual information estimation, our method is competitive with the state-of-the-art method and in Variational Bayesian application, our method stabilizes training of MNIST dataset leading to sharp reconstruction.

2 Related Work

Nguyen et al. [1] used variational method to estimate KL divergence from samples of two distribution using convex risk minimization (CRM). They used the RKHS norm as a way to both measure and penalize the complexity of the variational function. However, their work required handling all data at once and solving a convex optimization problem which has time complexity in the order of $O(m^3)$ and space complexity in the order of $O(m^2)$. Ahuja [11] used similar convex formulation in RKHS space and found it difficult to scale. VDM reformulated the f-Divergence objective using Fenchel duality and used a neural network to represent the variational function [6]. Although close in concept to [1], it is scalable since it uses a separate discriminator network and adversarial optimization. It, however, did not control the complexity of the neural-net function, and faced issues with stability.

One area of modern application of KL-divergence estimation is in computing mutual information, which is useful in applications such as stabilizing GANs [7]. MINE [7] also optimized a lower bound to KL divergence (Donsker-Varadhan representation). Similar to VDM, MINE used a neural network as the dual variational function: it is thus scalable, but without complexity control and is unstable. Another use of KL divergence is scalable variational inference (VI) as shown in AVB [8]. VI requires KL divergence estimation between the posterior and the prior, which becomes nontrivial when a sample based scalable estimation is required. AVB solved it using GAN-type adversarial formulation and a neural network discriminator. Similarly, [5] used GAN-type adversarial formulation to obtain KL divergence in amortized inference.

Chen et al. [2] proposed TC-VAE to improve disentanglement by penalizing the KL divergence between the marginal latent distribution and the product of marginals in each dimension. The KL divergence was computed by a minibatch-based sampling strategy that gives a biased estimate. Our work is close to Song et al. [9] who investigated the high variance in existing mutual information estimators and found that clipping the discriminator output is helpful in reducing variance. In our work, we take a principled way to connect variance to the complexity of discriminator function space and constrain it by penalizing its RKHS norm instead. None of the existing works considered
looking at the discriminator function space, connecting its complexity to the unreliable KL-divergence estimation, or mitigating the problem by controlling the complexity.

3 Reproducing Kernel Hilbert Space

Let $\mathcal{H}$ be a Hilbert space of functions $f : \mathcal{X} \rightarrow \mathbb{R}$ defined on non-empty space $\mathcal{X}$. It is a Reproducing Kernel Hilbert Space (RKHS) if the evaluation functional, $\delta_{x} : \mathcal{H} \rightarrow \mathbb{R}$, $\delta_{x} : f \mapsto f(x)$, is linear continuous $\forall x \in \mathcal{X}$. Every RKHS, $\mathcal{H}_K$, is associated with a unique positive definite kernel, $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, called the reproducing kernel [12], such that it satisfies:

1. $\forall x \in \mathcal{X}, K(., x) \in \mathcal{H}_K$
2. $\forall x \in \mathcal{X}, \forall f \in \mathcal{H}_K$, $\langle f, K(., x) \rangle_{\mathcal{H}_K} = f(x)$

RKHS is often studied using a specific integral operator. Let $\mathcal{L}_2(d\rho)$ be a space of functions $f : \mathcal{X} \rightarrow \mathbb{R}$ that are square integrable with respect to a Borel probability measure $d\rho$ on $\mathcal{X}$, we define an integral operator $\mathcal{L}_K : \mathcal{L}_2(d\rho) \rightarrow \mathcal{L}_2(d\rho)$ [13, 14]:

\[
(\mathcal{L}_K f)(x) = \int_{\mathcal{X}} f(y) K(x, y) d\rho(y)
\]

This operator will be important in constructing a function in RKHS and in computing sample complexity.

4 Problem Formulation and Contribution

GAN-type Objective for KL Estimation: Let $p(x)$ and $q(x)$ be two probability density functions in space $\mathcal{X}$ and we want to estimate their KL divergence using finite samples from each distribution in a scalable and minibatch compatible manner. As shown in [8, 5], this can be achieved by using a discriminator function. First, a discriminator $f : \mathcal{X} \rightarrow \mathbb{R}$ is trained with the objective:

\[
f^* = \arg\max_{f} [E_{p(x)} \log \sigma(f(x)) + E_{q(x)} \log(1 - \sigma(f(x)))]
\]

where $\sigma$ is the Sigmoid function given by $\sigma(x) = \frac{e^x}{1+e^x}$. Then it can be shown [8, 5] that the KL divergence $KL(p(x)\|q(x))$ is given by:

\[
KL(p(x)\|q(x)) = E_{p(x)}[f^*(x)]
\]

Sources of Error: Eq. (1) is ambiguous in the sense that it is silent about the discriminator function space over which the optimization is carried out. Typically, a neural network is used as the discriminator. This implies that we are considering the space of functions represented by the neural network of given architecture as the hypothesis space, over which the maximization occurs in eq. (1). Hence, we must rewrite eq. (1) as

\[
f^*_h = \arg\max_{f \in h} [E_{p(x)} \log \sigma(f(x)) + E_{q(x)} \log(1 - \sigma(f(x)))]
\]

where $h$ is the discriminator function space. Furthermore, we also approximate integrals in eq. (2) with the Monte Carlo estimate using finite number of samples, say $m$, from the distribution $p$ and $q$.

\[
f^*_m = \arg\max_{f \in h} \left[ \frac{1}{m} \sum_{x_i \sim p(x)} \log \sigma(f(x_i)) + \frac{1}{m} \sum_{x_j \sim q(x)} \log(1 - \sigma(f(x_j))) \right]
\]

Similarly, we write KL estimate obtained from, respectively, infinite and finite samples as:

\[
KL(f) = E_{p(x)}[f(x)], \quad KL_m(f) = \frac{1}{m} \sum_{x_i \sim p(x)} [f(x)]
\]

Each of these steps introduce some error in our estimate. We can now start our analysis by first decomposing the total estimation error as:

\[
KL_m(f^*_m) - KL(f^*) = KL_m(f^*_m) - KL(f^*_h) + KL(f^*_h) - KL(f^*_m) + KL(f^*_m) - KL(f^*)
\]

Deviation-from-mean error Discriminator induced error Bias

This equation decomposes total estimation error into three terms: 1) deviation from the mean error, 2) error in KL estimate by the discriminator due to using finite samples in optimization eq. (3), and 3) bias when the considered function space does not contain the optimal function. Here, we concentrate on quantifying the probability of deviation-from-mean error which is directly related to observed variance of the KL estimate.
Summary of Technical Contributions: Since the deviation is the difference between a random variable and its mean, we can bound the probability of this error using concentration inequality and the complexity of the function space of \( f^\theta \). To use smooth function space, we propose to construct a function out of neural networks such that it lies on RKHS (Section 5). Then, we bound the probability of deviation-from-mean error through the covering number of the RKHS space (Section 6.1), then control complexity (Section 6.2) and prove consistency of the proposed estimator (Section 7).

5 Constructing \( f \) in RKHS

The following theorem due to [15] paves a way for us to construct a neural function in RKHS.

**Theorem 1.** ([15] Appendix A) A function \( f \in \mathcal{L}_2(dp) \) is in Reproducing Kernel Hilbert Space, \( \mathcal{H}_K \), if and only if it can be expressed as

\[
\forall x \in \mathcal{X}, f(x) = \int_{\mathcal{W}} g(w) \psi(x, w) d\tau(w), \tag{6}
\]

for a certain function \( g : \mathcal{W} \to \mathbb{R} \) such that \( ||g||^2_{\mathcal{L}_2(dp)} < \infty \). The RKHS norm of \( f \) satisfies

\[
||f||^2_{\mathcal{H}_K} \leq ||g||^2_{\mathcal{L}_2(dp)} \text{ and the kernel } K \text{ is given by}
\]

\[
K(x, t) = \int_{\mathcal{W}} \psi(x, w) \psi(t, w) d\tau(w) \tag{7}
\]

Theorem [1] not only gives us a condition when a square integrable function is guaranteed to lie in RKHS, it also provides us with a recipe to construct a function in RKHS. We use this theorem with the neural networks as \( \psi \) and \( g \). We sample \( w \sim \mathcal{N}(0, \gamma I) \) and pass it through two neural networks, \( \psi \) and \( g \), where \( \psi \) takes \( x \) and \( w \) as two arguments and \( g \) takes only \( w \) as an argument. More precisely, we consider \( \psi(x, w) = \phi_\theta(x)^T w \). The kernel \( K \), as defined in eq. (7), can be obtained as:

\[
K_\theta(x^*, t^*) = \int_{\mathcal{W}} \phi_\theta(x^*)^T w u^T \phi_\theta(t^*) d\tau(u) = \gamma \phi_\theta(x^*)^T \phi_\theta(t^*) \tag{8}
\]

where \( E_{w \sim \mathcal{N}(0, \gamma I)}[w u^T] = \gamma 1 \). We sometimes denote the kernel \( K \) by \( K_\theta \) to emphasize that it is a function of neural network parameters, \( \theta \).

Traditionally, kernel \( K \) remains fixed and the norm of the function \( f \) determines the complexity of the function space. In our formulation, both the RKHS kernel and its norm with respect to the kernel change during training since the kernel depends on neural network parameters, \( \theta \). Therefore, the challenge is to tease out how neural parameters, \( \theta \), affect the deviation-from-mean error in eq. (5).

6 Error Analysis and Control

**Assumptions:** Before starting our analysis, we list assumptions upon which our theory is based.

- **A1:** The input domains \( \mathcal{X} \) and \( \mathcal{W} \) are compact.
- **A2:** The functions \( \phi_\theta \) and \( g \) are Lipschitz continuous with Lipschitz constants \( L_\phi \) and \( L_g \) respectively.
- **A3:** Higher order derivatives \( D^\tau_\phi K(x, t) \) up to some high order \( \tau = h/2 \) of kernel \( K \) exist.

Assumptions A1 is satisfied in our experiments since we consider a bounded set in \( \mathbb{R}^n \) and \( \mathbb{R}^D \) as our domains. Similarly, A2 is satisfied since we enforce Lipschitz continuity of \( \phi \) and \( g \) by using spectral normalization [16]. Assumption A3 is a bit subtle. By the definition of \( K \) in eq. (8), higher order derivative of \( K \) exists if higher order derivative of \( \phi_\theta \) exists. This is readily satisfied by deep networks with smooth activation functions, and is true everywhere except at origin for ReLU activation. Using the boundedness of the input domain and Lipschitz continuity, we show the following:

**Proposition 1.** Under the assumptions A1, A2, we have \( \sup_{K_\theta} K_\theta(x, t) < \infty \) and \( ||g||^2_{\mathcal{L}_2(dp)} < \infty \).

6.1 Bounding the Error Probability of KL Estimates

Bounding the probability of deviation-from-mean error (eq. (5)) is tricky since, in our case, the kernel is not fixed and we are also optimizing over them. We bound it in two steps: 1) we derive a bound for a fixed kernel, 2) we take supremum of this bound over all the kernels parameterized by \( \theta \).
For a fixed kernel, we first bound the probability of deviation-from-mean error in terms of the covering number in Lemma [1]. We then use an estimate of the covering number of RKHS due to [14] to relate the bound to kernel $K_{\theta}$ in Theorem 2 identifying the role of neural networks in this error bound.

**Lemma 1.** Let $f_{H_K}^m$ be the optimal discriminator function in an RKHS $H_K$ which is $M$-bounded. Let $KL_m(f_{H_K}^m) = \frac{1}{m} \sum_{i=1}^m f_{H_K}^m(x_i)$ and $KL(f_{H_K}^m) = \mathbb{E}_{p(x)}[f_{H_K}^m(x)]$ be the estimate of KL divergence from $m$ samples and that by using the true distribution $p(x)$ respectively. Then the probability of error at some accuracy level, $\epsilon$, is lower-bounded as:

$$\text{Prob}(|KL_m(f_{H_K}^m) - KL(f_{H_K}^m)| \leq \epsilon) \geq 1 - 2N(H_K, \frac{\epsilon}{4\sqrt{M^2}}) \exp(-\frac{m\epsilon^2}{4M^2})$$

where $N(H_K, \eta)$ denotes the covering number of an RKHS $H_K$ with disks of radius $\eta$, and $S_K = \sup_{x,t} K(x,t)$ which we refer to as kernel complexity.

**Proof Sketch.** We cover RKHS with discs of radius $\eta = \frac{\epsilon}{4\sqrt{M^2}}$. Within this radius, the deviation does not change too much. So, we can bound deviation probability at the center of disc and apply union bound over all the discs. To bound deviation probability at the center, we apply Hoeffding’s inequality and applying union bound simply leads to counting number of discs which is exactly the covering number. See supplementary materials for the full proof.

Lemma 1 bounds the probability of error in terms of the covering number of the RKHS space. Note the radius of the disc is inversely related to $S_K$ which indicates how complex the RKHS space defined by the kernel $K_{\theta}$ is. Here $K_{\theta}$ depends on the neural network parameters $\theta$. Therefore, we denote $S_K$ as a function of $\theta$ as $S_K(\theta)$ and term it kernel complexity. Next, we use Lemma 2 due to [14] to obtain an error bound in estimating KL divergence with finite samples in Theorem 2.

**Lemma 2 (14).** Let $K: X \times X \to \mathbb{R}$ be a $C^\infty$ Mercer kernel and the inclusion $I_K : H_K \to C(X)$ be the compact embedding defined by $K$ to the Banach space $C(X)$. Let $B_R$ be the ball of radius $R$ in RKHS $H_K$. Then $\forall \eta > 0, R > 0, h > n$, we have

$$\ln N(I_K(B_R), \eta) \leq \left( \frac{R C_h}{\eta} \right)^{2n}$$

(9)

where $N$ gives the covering number of the space $I_K(B_R)$ with discs of radius $\eta$, and $n$ represents the dimension of the input space $X$. $C_h$ is given by $C_h = C_s \sqrt{||Z_s||}$ where $Z_s$ is a linear embedding from square integrable space $L_2(d\rho)$ to the Sobolev space $H^{h/2}$ and $C_s$ is a constant.

To prove Lemma 2, the RKHS space is embedded in the Sobolev Space $H^{h/2}$ using $Z_s$ and then the covering number of the RKHS space is used. Thus the norm of $Z_s$ and the degree of Sobolev space, $h/2$, appears in the covering number of a ball in $H^h$. In Theorem 2, we use Lemma 1 and 2 to bound the estimation error of KL divergence.

**Theorem 2.** Let $KL(f_{H_K}^m)$ and $KL_m(f_{H_K}^m)$ be the estimates of KL divergence obtained by using true distribution $p(x)$ and $m$ samples respectively as described in Lemma 1, then the probability of error in the estimation at the error level $\epsilon$ is given by:

$$\text{Prob}(|KL_m(f_{H_K}^m) - KL(f_{H_K}^m)| \leq \epsilon) \geq 1 - 2 \exp\left[\left(\frac{4R C_p \sqrt{S_p} ||Z_p||}{\epsilon}\right)^{\frac{2n}{\eta}} - \frac{m\epsilon^2}{4M^2}\right]$$

where $C_p \sqrt{S_p} ||Z_p|| = \sup_{K_{\theta}} C_s \sqrt{S_K(\theta)} ||Z_s||$, i.e. $C_p, S_p, Z_p$ correspond to a kernel for which the bound is maximum.

**Proof.** We prove this in two steps: First we obtain an error bound for a fixed kernel space and apply supremum over all $\theta$. For any RKHS $H_{K_{\theta}}$, with fixed kernel $K_{\theta}$, we have

$$\text{Prob}(|KL_m(f_{H_{K_{\theta}}}^m) - KL(f_{H_{K_{\theta}}}^m)| \geq \epsilon) \leq 2 \exp\left[\left(\frac{4R C_s \sqrt{S_K(\theta)} ||Z_s||}{\epsilon}\right)^{\frac{2n}{\eta}} - \frac{m\epsilon^2}{4M^2}\right]$$

(10)
We prove this error bound as follows. Lemma 2 gives the covering number of an RKHS ball of radius $R$, which we apply to Lemma 1. We fix the radius of discs to $\eta = \frac{1}{4\sqrt{n}}$ in Lemma 1 and substitute $C_h = C_s \sqrt{||Z_s(\theta)||}$ to obtain eq. (10).

Since we are continuously changing $\theta$ during training, the kernel also changes. Hence, to find the upper bound over all possible kernels, we take the supremum over all kernels.

$$\text{Prob.}(|KL_m(f^m_H) - KL(f^m_H)| \geq \epsilon) \leq \sup_{K_\rho} \text{Prob.}(|KL_m(f^m_{HK_\rho}) - KL(f^m_{HK_\rho})| \geq \epsilon)$$

$$\leq 2 \exp \left[ \frac{4RC_p \sqrt{S_p ||L_p||}}{\epsilon} - \frac{mc^2}{4M^2} \right]$$

where $S_p = S_K(\theta_p)$ and $L_p = L_K(\theta_p)$, i.e., $S_p$ and $L_p$ correspond to kernel complexity and Sobolev operator norm corresponding to optimal kernel $K_{\theta_p}$ that extremizes eq. (11). Theorem statement readily follows from eq. (12).

Theorem 2 shows that the error increases exponentially with the radius of the RKHS space, $R$, complexity of the kernel $S_K(\theta_p)$, and the norm of the Sobolev space embedding operator $||L_p||$. The Sobolev embedding operator, $L_p$, is a mapping from $L_2(d\rho)$ to the Sobolev space $H^{h/2}$. It can be shown that the operator norm can be bounded as $||L_p|| \leq \rho(X) \sum_{|\alpha| \leq h/2} \sup_{x \in X} (D^\alpha \theta_p(x, t))^2$, where $\rho$ is the measure of the input space $X$. Therefore, the norm $||L_p||$ measures smoothness of $K_{\theta_p}$ in terms of norm of its derivative in addition to the supremum value of $R$, while $S_K(\theta_p)$ only depends on the supremum value of $K_{\theta_p}$.

### 6.2 Complexity Control

From Theorem 2, we see that the error probability could be decreased by decreasing $R$, $||L_p||$ and $S_K(\theta_p)$. Using argument similar to the proof of Proposition 1, we can show that the Lipschitz constraint on $\theta_q$ also affects $S_K$ and may affect $||L_p||$. In our experiments, however, we fix the Lipschitz constraints during optimization and do not change $S_K$ and $||L_p||$ dynamically. Here, we focus on the norm, $R$ from Theorem 2. To obtain the optimal discriminator $f^m_H$, we optimize the following objective with an extra penalization of the upper bound, i.e. $||g||$ on the RKHS norm of $f$:

$$f^m_H = \arg \max_{f \in H} \frac{1}{m} \sum_{x_i \sim p(x_i)} \log \sigma(f(x_i)) + \frac{1}{m} \sum_{x_j \sim q(x_j)} \log(1 - \sigma(f(x_j))) - \frac{\lambda_0}{m} ||g||^2_{L_2(d\tau)}$$

The regularization term prevents the radius of RKHS ball from growing, maintaining a low error probability. Optimization of eq. (13) w.r.t. neural network parameters $\theta$ allows dynamic control of the complexity of the discriminator function on the fly in a scalable and efficient way. Note that, computation of $||g||_{L_2(d\tau)}$ requires randomly sampling $w \sim \mathcal{N}(0, \gamma I)$ and passing through neural network $g$ independent of the data $x_i, x_j$. Therefore, if the computational complexity of optimization is $O(m)$, it will remain the same after incorporating this additional term, i.e. regularization does not increase asymptotic time complexity which is linear with the number of samples, $m$.

### 7 Variance and Consistency of the Estimate

#### 7.1 Variance Analysis

Theorem 2 gives an upper bound on the probability of error. Intuitively, the variance and probability of error behave similarly for many distributions, i.e. higher variance might indicate higher probability of error. Below we quantify this intuition for a Gaussian distributed estimate:

**Theorem 3.** Let $X = KL_m(f^m_H)$ be the estimated KL divergence using $m$ samples as described in Theorem 2. Assuming that $X$ follows a Gaussian distribution $X \sim \mathcal{N}(\mu, \sigma^2)$, we can obtain an upper bound on this variance of the estimate as follows:

$$\sigma \leq \epsilon \frac{\exp^{-1} \left[ -4 \exp \left( \frac{4RC_p \sqrt{S_p ||L_p||}}{\epsilon} - \frac{mc^2}{4M^2} \right) \right] + 1}{\text{erf}^{-1} \left( -\frac{\epsilon}{\sigma} \right)}$$

where erf is the Gauss error function and is a monotonic function.
Figure 1: a) Top scatter plot compares KL divergence estimates between a method using Neural network discriminator without complexity control (red) and that using RKHS discriminator with complexity control (blue); b) In the bottom, we show the effect of varying the regularization parameter $\lambda$ on bias and variance while using the RKHS discriminator with complexity control as in eq.(13).

Obviously, this relation applies only to Gaussian distributed estimate, a strong assumption. However, Theorem 3 is presented for illustrative purpose. It suggests that by decreasing $R$, the radius of the RKHS ball, the variance of the estimate could be decreased. Experimentally, we observe that the variance decreases as we penalize the RKHS norm more, consistent with the spirit of Theorem 3.

### 7.2 Consistency of Estimates

Here we show that the regularized objective leads to a consistent estimation.

**Theorem 4.** Let $f^*$ and $f^m$ be optimal discriminators as described in eq. (1) and eq. (13) respectively, and the KL estimate is given by $KL(f) = E_{p(x)}[f(x)]$, $KL_m(f) = \frac{1}{m} \sum_{x \sim p(x)} f(x)$. Then, in the limiting case as $m \to \infty$, $|KL_m(f^m) - KL(f^*)| \to 0$.

**Proof Sketch.** The difference between the true KL divergence and the estimated KL divergence can be divided into three terms as shown in eq. (5). We assume that our function space is rich enough to contain the true solution, driving bias to zero. From Theorem 2 we see that in the limiting case $m \to 0$, the deviation-from-mean error goes to 0. Therefore, the key step that remains to be shown is that the discriminator induced error (second term in eq.(5)) also goes to 0 as $m \to \infty$.

It can be shown if we can prove that the optimal discriminator in eq. (13) approaches the optimal discriminator in eq. (1). To prove this, we show that the argument being maximized by $f^m$ approaches the argument being maximized by $f^*$ in the limiting case. To show this, we need to show that the function space, $\log \sigma f$, is Glivenko Cantelli [17], which we prove in following steps:

1. We show that $f$ is Lipschitz continuous by definition and due to Lipschitz continuity of $\phi_B$. Then we show that $\log \sigma f$ is Lipschitz continuous if $f$ is Lipschitz continuous.
2. Then we show that for a class of functions with Lipschitz constant $L$, the metric entropy, $\log N$, can be obtained in terms of $L$ and entropy number of the bounded input space, $\mathcal{X}$.
3. Since the metric entropy does not grow with the number of samples $m$, we show that $\frac{1}{m} \log N \to 0$ which lets us show that $\log \sigma f$ belongs to Glivenko Cantelli class of functions by using Theorem 2.4.3 from [17]. See supplementary material for the complete proof.

### 8 Experimental Results

We present results on three applications of KL divergence estimation: 1. KL estimation between simple Gaussian distributions, 2. Mutual information estimation, 3. Variational Bayes. In our
experiments, the RKHS discriminator is constructed with $\psi$ and $g$ networks as described in Section 5, where the network $\psi$ is very close to a regular neural network. In two experiments, we compare our results with the models using regular neural net discriminator to ensure that the difference in performance between RKHS and regular neural network is not due to architectural difference.

**KL Estimation between Two Gaussians**  We assume that we have finite sets of samples from two distributions. We further assume that we are required to apply minibatch based optimization. We consider estimating KL divergence between two Gaussian distributions in 2D, where we know the analytical KL divergence between the two distributions as the ground truth. We consider three different pairs of distributions corresponding to true KL divergence values of 1.3, 13.8 and 38.29, respectively and use $m = 5000$ samples from each distribution to estimate KL in the finite case. We repeat the estimation experiments with random initialization 30 times and report the mean, standard deviation, scatter and box plots.

Fig. 1 top row compares the estimation of KL divergence with regular neural net and RKHS discriminator with complexity control based on eq. (13). With our proposed RKHS discriminator, the KL estimates are significantly more reliable and accurate: error reduced from 0.5 to 0.04, 5.8 to 1.07 and 60.6 to 9.7 and variance reduced from 0.2 to 0.002, 223 to 4.4 and 3521 to 33 for true KL 1.3, 13.8 and 38.29 respectively. In Fig. 1 bottom row, we investigate our complexity control method on the effect of varying the regularization parameter $\lambda = \lambda_0/m$. As expected, increasing regularization parameter penalizes more on the RKHS norm and therefore reduces variance. This is consistent with our theory. Regarding bias, however, as we increase the $\lambda$, the bias decreases and then starts to increase. Hence, one needs to strike a balance between bias and variance while choosing $\lambda$.

**Mutual Information Estimation**  Computation of mutual information is a direct use case of KL divergence computation. We replicate the experimental setup of [18, 9] to estimate mutual information between $(x, y)$ drawn from 20-d Gaussian distributions, where the mutual information is increased by step size of 2 from 2 to 10. We compare the performance of our method with traditional KL divergence computation methods like contrastive predictive coding (CPC) [18], convex risk minimization (NWJ) [1] and SMILE [9]. In Fig.2 our method with RKHS discriminator (with $\lambda = 1e^{-5}$) performs better than CPC [18] and NWJ [1], and is competitive with the state-of-the-art, SMILE [9]. In the bottom row, we also show the effect of regularization parameter $\lambda$ in our method. Similar to the previous experiment, increasing the regularization parameter decreases the variance and increases the bias. It is consistent with our theoretical insights about the effect of reducing RKHS norm on variance.

**Adversarial Variational Bayes** Variational Bayes requires KL divergence estimation. When we do not have access to analytical form of the posterior/prior distributions, but only have access to the samples, we need to estimate KL divergence from samples. Adversarial Variational Bayes (AVB) [8] presents a way to achieve this using a discriminator network. We adopt this setup and demonstrate that the training becomes unstable if we do not constrain the complexity of the discriminator. First, we
Figure 3: (a) Comparison of MNIST digit reconstruction using AVB autoencoder model [8]. Trace of KL divergence and reconstruction loss in AVB model with Neural network discriminator (b) and RKHS discriminator in (c).

Train AVB on MNIST dataset with a simple neural network discriminator architecture. As the training progresses, the KL divergence blows up after about 500 epochs (Fig. 3(b)) and the reconstruction starts to get worse (Fig. 3(a)). We modify the same architecture according to our construction such that it lies in RKHS and then penalize the RKHS norm as in eq. (13). It stabilizes the training for a large number of epochs and the reconstruction does not deteriorate as the training progresses, resulting into sharp reconstruction (Fig. 3(a)). We want to clarify that this instability in training neural net discriminator is present if we use a basic discriminator architecture. It does not mean that there exists no other method to design a stable neural net discriminator. In fact, AVB [8] presents a discriminator that adds additional inner product structure to stabilize the discriminator training. Our point here is that we can stabilize the training by ensuring that the discriminator lies in a well behaved function space (the RKHS) and controlling its complexity, consistent with our theory.

9 Limitations, Discussion and Conclusion

Limitations: The proposed construction of neural function in RKHS exhibits good properties of both the deep learning and kernel methods. However, it requires constructing two separate deep networks, $\psi$ and $g$. It makes our model a bit bulky and also requires more parameter due to additional $g$. Moreover, currently our RKHS discriminator’s output is scalar; generalizing this function to a multivariable output could make our model bulkier and increase parameters even more. Second limitation is the requirement of higher order derivative of kernel $K$ in assumption A3. While this requirement is satisfied if smooth activation function is used in $\phi_{\theta}$, for activations like ReLU or LeakyReLU, the derivatives exist everywhere except at the origin. In these cases, we need to carefully investigate if we can use subgradients to define operator norm $||L_p||$.

Discussion and Conclusion: We have shown that using a regular neural network as a discriminator in estimating KL divergence results in unreliable estimation if the complexity of the function space is not controlled. We then showed a solution by constructing a discriminator function in RKHS space using neural networks and penalizing its complexity in a scalable way. Although the idea to use RKHS norm to penalize complexity is not new (see for example [1]), it is not clear how to use this idea directly on the function $f$. In traditional kernel methods, algorithms often do not work with RKHS function $f$ directly, but rather work with kernel matrix, $K$ by using, for example, the Representer Theorem [20]. In the case of big data, working with the big kernel matrix is computationally expensive although some methods have been proposed to speed up the computation, like Random Fourier Feature [21]. We propose a different view by directly constructing a function in RKHS space,
which led us to scalable algorithm while incorporating the advantages of neural networks. Moreover, our representation could also be seen as an improvement over RFF by using neural basis, $\psi$, instead of Fourier basis. The idea of constructing a neural-net function in RKHS and complexity control could also be useful in stabilizing GANs in general. Currently, the most successful way to stabilize GANs is to enforce smoothness by gradient penalization \cite{22, 23, 24}. On the light of the present analysis, gradient penalty could also be thought as a way to control the complexity of the discriminator.

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A Problem Formulation and Contribution

**GAN-type Objective for KL Estimation** Let \( f \) be a discriminator, \( f : X \rightarrow \mathbb{R} \). Let \( p(x) \) and \( q(x) \) be two probability density functions defined over the space \( X \). First, we train a discriminator as:

\[
f^* = \arg\max_f [E_p(x) \log \sigma(f(x)) + E_q(x) \log(1 - \sigma(f(x)))]
\]

(15)

where \( \sigma \) is the Sigmoid function given by \( \sigma(x) = \frac{e^x}{1 + e^x} \). Then the KL divergence \( KL(p(x)||q(x)) \) is given by:

\[
KL(p(x)||q(x)) = E_p(x) [f^*(x)]
\]

(16)

**Proof.** The proof is based on similar proofs in [8, 5] and presented here for the sake of completeness. We rewrite the objective as:

\[
\int p(x) \log \sigma(f(x)) + q(x) \log(1 - \sigma(f(x))) \, dx
\]

(17)

This integral is maximum with respect to \( f \) if and only if the integrand is maximal for every \( x \). As argued in the Proposition 1 of [25], the function \( t \mapsto a \log(t) + b \log(1 - t) \) attains its maximum at \( t = \frac{a}{a+b} \) showing that,

\[
\sigma(f^*(x)) = \frac{p(x)}{p(x) + q(x)}
\]

(19)

Plugging the expression for Sigmoid function, we obtain,

\[
f^*(x) = \frac{p(x)}{q(x)}
\]

(20)

Therefore, by the definition of KL divergence, we have:

\[
KL(p(x)||q(x)) = E_p(x) [\frac{p(x)}{q(x)}] = E_p(x) [f^*(x)]
\]

(21)

\[\square\]

B Error Analysis and Control

We start with the set of assumptions based on which our theory is developed.

A1. The input domains \( \mathcal{X} \) and \( \mathcal{W} \) are compact.

A2. The functions \( \phi_\theta \) and \( g \) are Lipschitz continuous with Lipschitz constant \( L_\phi \) and \( L_g \) respectively.

A3. Higher order derivatives \( D_\alpha K(x,t) \) of kernel \( K \) exist up to some high order \( \tau = h/2 \).

**Proposition 2.** Under the assumptions A1, A2, we have

i) \( \sup_{x,t} K_\theta(x,t) < \infty \), and

ii) \( \|g\|_{L^2(d\tau)}^2 < \infty \).

**Proof.** i) By the definition \( K_\theta(x,t) = \gamma \langle \phi_\theta(x), \phi_\theta(t) \rangle \). Using Cauchy Schwartz,

\[
K_\theta(x,t) \leq \gamma \|\phi_\theta(x)\| \|\phi_\theta(t)\| \leq \gamma L_\phi \|x\| L_\phi \|t\| \leq \infty
\]

(22)

(23)

(24)
where we used the fact that $\mathcal{X}$ is bounded, and therefore, $\|x\|$ and $\|t\|$ are finite.

ii) By definition,

$$\|g\|^2_{L^2(dx)} = \int g(w)^2 d\tau(w)$$  \hspace{1cm} (25)

$$\leq \int L^2_w \|w\|^2 d\tau(w)$$ \hspace{1cm} (26)

$$= L^2_w tr(C_w)$$ \hspace{1cm} (27)

where $C_w$ is the uncentered covariance matrix of the Gaussian distributed $w$. Therefore, we immediately obtain $\|g\|^2_{L^2(dx)} < \infty$.

These results are useful in constructing a function $f$ in RKHS in Theorem 1 (Section 5) of the main paper.

**B.1 Bounding the Error Probability of KL Estimates**

We bound the deviation-from-mean error in two steps: 1) we derive a bound for a fixed kernel, 2) we take supremum of this bound over all the kernels parameterized by $\theta$.

For a fixed kernel, we first bound the probability of deviation-from-mean error in terms of the covering number in Lemma 1. Then, we use an estimate of the covering number of RKHS due to [14] to obtain a bound of error probability in terms of the kernel $K_{\theta}$ in Lemma 3. Note that, Lemma 3 is proved for a fixed kernel $K_{\theta}$, where $\theta$ is fixed. Then finally in Theorem 2, we take supremum over all kernels $K_{\theta}$ to obtain a bound on error probability on a space of functions with all possible kernels.

**Lemma 1.** Let $f^m_{\mathcal{H}_K}$ be the optimal discriminator function in a RKHS $\mathcal{H}_K$ which is $M$-bounded. Let $KL_m(f^m_{\mathcal{H}_K}) = \frac{1}{m} \sum_i f^m_{\mathcal{H}_K}(x_i)$ and $KL(f^m_{\mathcal{H}_K}) = E_{p(x)}[f^m_{\mathcal{H}_K}(x)]$ be the estimate of KL divergence from $m$ samples and that by using true distribution $p(x)$ respectively. Then the probability of error at some accuracy level, $\epsilon$, is lower-bounded as:

$$Prob. (|KL_m(f^m_{\mathcal{H}_K}) - KL(f^m_{\mathcal{H}_K})| \leq \epsilon) \geq 1 - 2N(\mathcal{H}_K, \epsilon, \frac{\epsilon}{4\sqrt{S_K}}) \exp(-\frac{m\epsilon^2}{4M^2})$$

where $N(\mathcal{H}_K, \eta)$ denotes the covering number of a RKHS space $\mathcal{H}_K$ with disks of radius $\eta$, and $S_K = \sup_{x,t} K(x, t)$ which we refer as kernel complexity.

**Proof.** Let $\ell_z(f) = E_{p(x)}[f(x)] - \frac{1}{m} \sum_i f(x_i)$ denotes the error in the estimate such that we want to bound $|\ell_z(f)|$. We have,

$$\ell_z(f_1) - \ell_z(f_2) = E_{p(x)}[f_1(x) - f_2(x)] - \frac{1}{m} \sum_i f_1(x_i) - f_2(x_i)$$

We know $E_{p(x)}[f_1(x) - f_2(x)] \leq ||f_1 - f_2||_{\infty}$ and $\frac{1}{m} \sum_i f_1(x_i) - f_2(x_i) \leq ||f_1 - f_2||_{\infty}$. Using the triangle inequality, we obtain $|\ell_z(f_1) - \ell_z(f_2)| \leq 2||f_1 - f_2||_{\infty}$. Now, consider $f \in \mathcal{H}_K$, then,

$$|f(x)| = |\langle K_x, f \rangle| \leq ||f|| ||K_x|| = ||f|| \sqrt{K(x, x)}$$ \hspace{1cm} (28)

This implies the RKHS space norm and $\ell_\infty$ norm of a function are related by

$$||f||_\infty \leq \sqrt{S_K} ||f||_{\mathcal{H}_K}$$ \hspace{1cm} (29)

Hence, we have:

$$|\ell_z(f_1) - \ell_z(f_2)| \leq 2\sqrt{S_K} ||f_1 - f_2||_{\mathcal{H}_K}$$ \hspace{1cm} (30)

The idea of the covering number is to cover the whole RKHS space $\mathcal{H}_K$ with disks of some fixed radius $\eta$, which helps us bound the error probability in terms of the number of such disks. Let $N(\mathcal{H}_K, \eta)$ be such disks covering the whole RKHS space. Then, for any function $f$ in $\mathcal{H}_K$, we can find some disk, $D_j$ with centre $f_j$, such that $||f - f_j||_{\mathcal{H}_K} \leq \eta$. If we choose $\eta = \frac{\epsilon}{2\sqrt{S_K}}$, then from eq. (30), we obtain,

$$\sup_{f \in D_j} |\ell_z(f)| \geq 2\epsilon \implies |\ell_z(f_j)| \geq \epsilon$$ \hspace{1cm} (31)
Using the Hoeffding’s inequality, \( \text{Prob.}(|\ell_z(f_j)| \geq \epsilon) \leq 2e^{-\frac{m\epsilon^2}{2M^2}} \) and eq. (31),

\[
\text{Prob.}(\sup_{f \in \mathcal{B}_j} |\ell_z(f)| \geq 2\epsilon) \leq 2e^{-\frac{m\epsilon^2}{2M^2}}
\]  
(32)

Applying union bound over all the disks, we obtain,

\[
\text{Prob.}(\sup_{f \in \mathcal{H}} |\ell_z(f)| \geq 2\epsilon) \leq 2N(\mathcal{H}, \frac{\epsilon}{2\sqrt{S_K}})e^{-\frac{m\epsilon^2}{2M^2}}
\]
(33)

\[
\text{Prob.}(\sup_{f \in \mathcal{H}} |\ell_z(f)| \leq \epsilon) \geq 1 - 2N(\mathcal{H}, \frac{\epsilon}{4\sqrt{S_K}})e^{-\frac{m\epsilon^2}{4M^2}}
\]

which proves the lemma.

On M-boundedness of \( f_{H_K}^m \)
To prove the lemma, we assumed that \( f_{H_K}^m \) is bounded. To see why this is reasonable, from eq. (29) we have \( ||f_{H_K}^m||_{\infty} \leq \sqrt{S_K}||f_{H_K}^m||_{H_K} \leq \sqrt{S_K}||g||_{\mathcal{L}_2(dp)} \). Therefore, \( f_{H_K}^m \) is bounded if \( S_K \) and \( ||g||_{\mathcal{L}_2(dp)} \) are bounded, which is true by Proposition 1.

**Remark 1.** We derived the error bound based on the Hoeffding’s inequality by assuming that our only knowledge about \( f \) is that it is bounded. If we have other knowledge, for example, if we know the variance of \( f \), we could use Bernstein’s inequality instead of Hoeffding’s inequality with minimal change to the proof. To the extent we are interested in the contribution of neural network in error bound, however, there is not much gain by using one inequality or the other. Hence, we stick with Hoeffding’s inequality and note other possibilities.

**Remark 2.** Note that in Lemma 1, the radius of disks are inversely related to the quantity, \( S_K \), meaning that if \( S_K \) is high, we would need large number of disks to fill the RKHS space. Hence, it denotes a quantity that reflects the complexity of the RKHS space. We, therefore, term it kernel complexity. Also in eq. (29) and the discussion about the M-boundedness, we see that the maximum value \( |f(x)| \) depends on \( S_K \), again providing insight into how \( S_K \) may control both maximum fluctuation and the boundedness.

Lemma 1 bounds the probability of error in terms of the covering number of the RKHS space. Next, we use Lemma 2 due to [14] to obtain an error bound in estimating KL divergence with finite samples in Theorem 2.

**Lemma 2 ([14]).** Let \( K : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) is a \( C^\infty \) Mercer kernel and the inclusion \( I_K : \mathcal{H}_K \to \mathcal{C}(\mathcal{X}) \) is the compact embedding defined by \( K \) to the Banach space \( \mathcal{C}(\mathcal{X}) \). Let \( B_R \) be the ball of radius \( R \) in RKHS \( \mathcal{H}_K \). Then \( \forall \eta > 0, R > 0, h > n, \) we have

\[
\ln N(I_K(B_R), \eta) \leq \left( \frac{RC_h}{\eta} \right)^{2n}
\]
(34)

where \( N \) gives the covering number of the space \( I_K(B_R) \) with disks of radius \( \eta \), and \( n \) represents the dimension of inputs space \( \mathcal{X} \). \( C_h \) is given by

\[
C_h = C\sqrt{||L_K||}
\]
(35)

where \( L_K \) is a linear embedding from square integrable space \( \mathcal{L}_2(dp) \) to the Sobolev space \( H^{h/2} \) and \( C \) is a constant.

To prove Lemma 2 the RKHS space is embedded in the Sobolev Space \( H^{h/2} \) using \( L_K \) and then covering number of Sobolev space is used. Thus the norm of \( L_K \) and the degree of Sobolev space, \( h/2 \), appears in the covering number of a ball in \( \mathcal{H}_K \). In Lemma 3 we use this Lemma to bound the estimation error of KL divergence.

**Lemma 3.** Let \( KL(f_{H_{K_0}}^m) \) and \( KL(f_{H_{K_0}}^m) \) be the estimates of KL divergence obtained by using true distribution \( p(x) \) and \( m \) samples respectively and using a fixed kernel, \( K_0 \) as described in Lemma 1 then the probability of error in the estimation at the error level \( \epsilon \) is given by:

\[
\text{Prob.}( |KL_m(f_{H_{K_0}}^m) - KL(f_{H_{K_0}}^m)| \geq \epsilon) \leq 2 \exp \left[ -\frac{ARC_s \sqrt{S_K(\theta)||Z_2(\theta)||}}{\epsilon} \right] - \frac{m\epsilon^2}{4M^2}
\]
Proof. Lemma 2 gives the covering number of a ball of radius $R$ in an RKHS space. In Lemma 1, if we consider the hypothesis space to be a ball of radius $R$, we can apply Lemma 2 in it. Additionally, since we fix the radius of disks to be $\eta = \frac{\epsilon}{4\sqrt{\delta_n}}$ in Lemma 1, we obtain,

$$
\text{Prob.}(|KL_m(f^m_{H_{K_\theta}}) - KL(f^m_{H_{K_\theta}})| \geq \epsilon) \leq 2 \exp \left[ - \frac{4\sqrt{S_{K_\theta}}RC_h}{\epsilon} \right] - \frac{m\epsilon^2}{4\delta_n^2}
$$

Substituting $C_h = C\sqrt{\|Z_{K_\theta}\|}$, we obtain,

$$
\text{Prob.}(|KL_m(f^m_{H_{K}}) - KL(f^m_{H_{K}})| \geq \epsilon) \leq 1 - 2 \exp \left[ - \frac{4RC\sqrt{S_{K_\theta}}\|Z_{K_\theta}\|}{\epsilon} \right] - \frac{m\epsilon^2}{4\delta_n^2}
$$

where $C_{\text{p}}\sqrt{S_p}\|Z_p\| = \sup_{K_\theta} C_s\sqrt{S_K(\theta)}\|Z_{\theta}\|$, i.e. $C_{\text{p}}, S_p, Z_p$ correspond to a kernel for which the bound is maximum.

Proof. Lemma 3 gives an error bound for a fixed kernel, $K_\theta$. To find an upper bound over all possible kernels, we take the supremum over all kernels.

$$
\text{Prob.}(|KL_m(f^m_{H_{K}}) - KL(f^m_{H_{K}})| \geq \epsilon) \leq \sup_{K_\theta} \text{Prob.}(|KL_m(f^m_{H_{K_\theta}}) - KL(f^m_{H_{K_\theta}})| \geq \epsilon) \leq 2 \exp \left[ - \frac{4RC_p\sqrt{S_p}\|Z_p\|}{\epsilon} \right] - \frac{m\epsilon^2}{4\delta_n^2}
$$

where $S_p = S_K(\theta_p)$ and $Z_p = Z_K(\theta_p)$, i.e., $S_p$ and $Z_p$ correspond to kernel complexity and Sobolev operator norm corresponding to optimal kernel $K_{\theta_p}$ that extremizes eq. (38). Theorem statement readily follows from eq. (39). \qed

C Variance and Consistency of the Estimate

C.1 Variance Analysis

Theorem 3. Let $X = KL_m(f^m_{H_{K}})$ be the estimated KL divergence using $m$ samples as described in Theorem 2. Assuming that $X$ follows a Gaussian distribution $X \sim \mathcal{N}(\mu, \sigma)$, we can obtain an upper bound on this variance of the estimate as follows:

$$
\sigma \leq \frac{\epsilon}{\sqrt{2\text{erf}^{-1} \left[ - 4 \exp \left[ - \frac{4RC_{\text{p}}\sqrt{S_p}\|Z_p\|}{\epsilon} \right] - \frac{m\epsilon^2}{4\delta_n^2} \right] + 1}}
$$

where erf is the Gauss error function

$$
\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt
$$

and it is a monotonic function.
Proof. $X$ follows a Gaussian distribution with mean $\mu$ and variance $\sigma$. Let its cumulative distribution function be $\Phi_{\mu, \sigma}$. By definition,

$$P(X \leq \hat{x}) = \Phi_{\mu, \sigma}(\hat{x})$$

(42)

$$P(X \geq \hat{x}) = 1 - \Phi_{\mu, \sigma}(\hat{x})$$

(43)

$$P(X - \mu \geq \epsilon) = 1 - \Phi_{\mu, \sigma}(\mu + \epsilon)$$

(44)

Since two sided probability is higher than one sided, we have,

$$P(X - \mu \geq \epsilon) \leq P(|X - \mu| \geq \epsilon)$$

(45)

$$\leq 2 \exp \left[\left(\frac{4RC_s \sqrt{S_K ||Z||}}{\epsilon}\right)^\frac{2\epsilon}{\sigma} - \frac{m\epsilon^2}{4M^2}\right]$$

(46)

where we used Theorem 2. Using eq\textsuperscript{44}, we have,

$$1 - \Phi_{\mu, \sigma}(\mu + \epsilon) \leq 2 \exp \left[\left(\frac{4RC_s \sqrt{S_K ||Z||}}{\epsilon}\right)^\frac{2\epsilon}{\sigma} - \frac{m\epsilon^2}{4M^2}\right]$$

(47)

For a Gaussian distribution, we can use the following expression for the cumulative distribution function,

$$\Phi_{\mu, \sigma}(\hat{x}) = \frac{1}{2} \left[1 + \text{erf}\left(\frac{\hat{x} - \mu}{\sigma \sqrt{2}}\right)\right]$$

(48)

where erf is the Gauss error function. Using this in the eq\textsuperscript{47},

$$1 - \text{erf}\left(\frac{\epsilon}{\sigma \sqrt{2}}\right) \leq 4 \exp \left[\left(\frac{4RC_s \sqrt{S_K ||Z||}}{\epsilon}\right)^\frac{2\epsilon}{\sigma} - \frac{m\epsilon^2}{4M^2}\right]$$

(49)

$$\text{erf}\left(\frac{\epsilon}{\sigma \sqrt{2}}\right) \geq -4 \exp \left[\left(\frac{4RC_s \sqrt{S_K ||Z||}}{\epsilon}\right)^\frac{2\epsilon}{\sigma} - \frac{m\epsilon^2}{4M^2}\right] + 1$$

(50)

Since the function erf is invertible within domain (-1,1), we have,

$$\frac{\epsilon}{\sigma \sqrt{2}} \geq \text{erf}^{-1}\left[-4 \exp \left[\left(\frac{4RC_s \sqrt{S_K ||Z||}}{\epsilon}\right)^\frac{2\epsilon}{\sigma} - \frac{m\epsilon^2}{4M^2}\right] + 1\right]$$

(51)

$$\sigma \leq \sqrt{2}\text{erf}^{-1}\left[-4 \exp \left[\left(\frac{4RC_s \sqrt{S_K ||Z||}}{\epsilon}\right)^\frac{2\epsilon}{\sigma} - \frac{m\epsilon^2}{4M^2}\right] + 1\right]$$

(52)

\textbf{C.2 Consistency of Estimates}

\textbf{Theorem 4.} Let $f^*$ and $f^m$ and $f^*_h$ be optimal discriminators defined as

$$f^* = \text{argmax}_{f} \left[ E_{p(x)} \log \sigma(f(x)) + E_{q(x)} \log(1 - \sigma(f(x))) \right]$$

(53)

$$f^*_h = \text{argmax}_{f} \left[ E_{p(x)} \log \sigma(f(x)) + E_{q(x)} \log(1 - \sigma(f(x))) \right]$$

(54)

$$f^m = \text{argmax}_{f} \left[ \frac{1}{m} \sum_{x_i \sim p(x)} \log \sigma(f(x_i)) + \frac{1}{m} \sum_{x_j \sim q(x_j)} \log(1 - \sigma(f(x_j))) \right] - \frac{\lambda}{m} \|g\|_2^2$$

(55)

and the KL estimate is given by $KL(f) = E_{p(x)}[f(x)]$, $KL_m(f) = \frac{1}{m} \sum_{x_i \sim p(x)} |f(x)|$. Then, in the limiting case as $m \to \infty$, $|KL_m(f^m) - KL(f^*)| \to 0$. 

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Proof. Estimation error can be divided into three terms as

\[
KL_m(f^m_h) - KL(f^*) = KL_m(f^m_h) - KL(f^*_h) + KL(f^*_h) - KL(f^*_h) + KL(f^*_h) - KL(f^*)
\]

Deviation-from-mean error Discriminator induced error Bias

Therefore,

\[
|KL_m(f^m_h) - KL(f^*)| \leq |KL_m(f^m_h) - KL(f^*_h)| + |KL(f^*_h) - KL(f^*_h)| + |KL(f^*_h) - KL(f^*)|
\]

(56)

To show that the total error goes to zero, we show that each term on the right goes to zero. The last term is the bias and we assume that the RKHS space \( h = \mathcal{H} \) we consider consists the true solution, \( f^* \). Hence the bias goes to zero.

Using Theorem 2, it is immediately clear that the first term, \( |KL_m(f^m_h) - KL(f^*_h)| \) approaches zero in the limiting case as \( m \to \infty \).

The only remaining is the second term, \( |KL(f^*_h) - KL(f^*_h)| \). In Theorem 5, we show that this term also goes to zero as \( m \to 0 \).

\[\square\]

**Theorem 5.** Let \( f^*_m \) and \( f^*_h \) be the optimal discriminators as defined in eq. (54) and eq. (55), and the KL divergence estimate using discriminators learned using finite and infinite samples be \( KL(f^m_h) = \int [f^m_h(x)] p(x) dx \) and \( KL(f^*_h) = \int [f^*_h(x)] p(x) dx \), where, Then, in the limiting case, we have

\[
\lim_{m \to \infty} |KL(f^m_h) - KL(f^*_h)| = 0
\]

**Proof.**

\[
|KL(f^m_h) - KL(f^*_h)| = |\int [f^m_h(x) - f^*_h(x)] p(x) dx|
\]

\[
\leq \sup_x |f^m_h(x) - f^*_h(x)| = \| f^m_h(x) - f^*_h(x) \|_\infty
\]

Therefore, we can show \( \lim_{m \to \infty} KL(f^m_h) - KL(f^*_h) = 0 \) if \( \lim_{m \to \infty} \| f^m_h(x) - f^*_h(x) \|_\infty = 0 \), that is, if the function \( f^m_h(x) \) converges uniformly to function \( f^*_h(x) \) in the limiting case.

The two maximizer functions are given by

\[
f^*_h = \arg\max_{f \in h} [E_{p(x)} \log \sigma(f(x)) + E_{q(x)} \log(1 - \sigma(f(x)))]
\]

(58)

\[
f^m_h = \arg\max_{f \in h} \left[ \frac{1}{m} \sum_{x_i \sim p(x_i)} \log \sigma(f(x_i)) + \frac{1}{m} \sum_{x_j \sim q(x_j)} \log(1 - \sigma(f(x_j))) \right] - \frac{\lambda_0}{m} ||g||^2
\]

(59)

As a first step in showing that \( f^m_h \) uniformly approaches \( f^*_h \), we first show that \( \lim_{m \to \infty} \frac{\lambda_0}{m} ||g||^2 = 0 \) in Lemma 3.

Then, to prove the rest, let us denote,

\[
G_m(f) = \frac{1}{m} \sum_{x_i \sim p(x_i)} \log \sigma(f(x_i)) + \frac{1}{m} \sum_{x_j \sim q(x_j)} \log(1 - \sigma(f(x_j)))
\]

\[
G(f) = E_{p(x)} \log \sigma(f(x)) + E_{q(x)} \log(1 - \sigma(f(x))
\]

In Lemma 5, we prove that functionals \( G(f) \) and \( G_m(f) \) are concave with respect to function \( f \). In the light of these two lemmas, we argue

\[
\lim_{m \to \infty} ||f^m_h(x) - f^*_h(x)||_\infty = 0 \text{ if } \lim_{m \to \infty} \sup_f |G_m(f) - G(f)| = 0
\]

(60)
Next, we show \( \lim_{m \to \infty} \sup_f |G_m(f) - G(f)| = 0 \) as follows. We have,

\[
|G_m - G| = \left| \frac{1}{m} \sum_{x_i \sim p(x)} \log \sigma(f(x_i)) + \frac{1}{m} \sum_{x_j \sim q(x)} \log(1 - \sigma(f(x_j))) \right| \\
- E_{p(x)} \log \sigma(f(x)) + E_{q(x)} \log(1 - \sigma(f(x))) \right| \\
\leq \left| \frac{1}{m} \sum_{x_i \sim p(x)} \log \sigma(f(x_i)) - E_{p(x)} \log \sigma(f(x)) \right| \\
+ \left| \frac{1}{m} \sum_{x_j \sim q(x)} \log(1 - \sigma(f(x_j))) - E_{q(x)} \log(1 - \sigma(f(x))) \right| \tag{61}
\]

\[
\therefore \lim_{m \to \infty} \sup_f |G_m(f) - G(f)| \leq \lim_{m \to \infty} \sup_f \left( \frac{1}{m} \sum_{x_i \sim p(x)} \log \sigma(f(x_i)) - E_{p(x)} \log \sigma(f(x)) \right) \\
+ \lim_{m \to \infty} \sup_f \left( \frac{1}{m} \sum_{x_j \sim q(x)} \log(1 - \sigma(f(x_j))) - E_{q(x)} \log(1 - \sigma(f(x))) \right) \tag{62}
\]

Both the terms on right hand side go to zero if \( \log \circ \sigma \circ f \) is in a Glivenko Cantelli class of functions using Empirical Process Theory \([17]\), which we prove in Lemma 6. That completes the proof. \( \square \)

**Lemma 4.** \( \lim_{m \to \infty} \frac{1}{m} \|g\|^2 = 0 \)

**Proof.** \( \|g\|_{L^2(p)} \) is bounded because \( g \) is Lipschitz continuous and its domain is bounded. Since, \( \|g\|_{L^2(p)} \) is bounded, we immediately obtain the required statement. \( \square \)

**Lemma 5.** The functional \( G(f) \) is concave with respect to function \( f \) in the following sense: \( \theta_1 G(f_1) + \theta_2 G(f_2) \leq G(\theta_1 f_1 + \theta_2 f_2) \) for any \( \theta_1, \theta_2 \in (0, 1) \) such that \( \theta_1 + \theta_2 = 1 \). The same is true for \( G_m(f) \).

**Proof.**

\[
\theta_1 G(f_1) + \theta_2 G(f_2) = \theta_1 \left[ \int p(x) \log \sigma(f_1(x)) dx + \int q(x) \log(1 - \sigma(f_1(x))) dx \right] \\
+ \theta_2 \left[ \int p(x) \log \sigma(f_2(x)) dx + \int q(x) \log(1 - \sigma(f_2(x))) dx \right] \tag{64}
\]

\[
= \int p(x) \left[ \theta_1 \log \sigma(f_1(x)) dx + \theta_2 \log \sigma(f_2(x)) dx \right] \\
+ \int q(x) \left[ \theta_1 \log \sigma(-f_1(x)) dx + \theta_2 \log \sigma(-f_2(x)) dx \right] \tag{65}
\]

\[
\leq \int p(x) \log \sigma(\theta_1 f_1(x) + \theta_2 f_2(x)) dx \\
+ \int q(x) \log \sigma[-(\theta_1 f_1(x) + \theta_2 f_2(x))] dx \tag{66}
\]

\[
= G(\theta_1 f_1 + \theta_2 f_2) \tag{67}
\]

where we used the fact that \( \log(1 - \sigma(f(x))) = \log \sigma(-f(x)) \) (this is straightforward using definition of Sigmoid function, \( \sigma \) in line 65). In line 66, we used the fact that \( \log \sigma \) is a concave function (see Lemma 5). \( \square \)

**Lemma 6.** \( \log \circ \sigma \circ f \) is a Glivenko Cantelli class of function.

**Proof.** In Lemma 7, we show that, by definition, \( f \) is Lipschitz continuous with some Lipschitz constant \( L_f \). In Lemma 8, we show that if \( f \) is a Lipschitz continuous function from \( \mathcal{X} \) to \( (-\infty, \infty) \) with Lipschitz constant, \( L_f \), then \( \log \sigma f \) is a function from \( \mathcal{X} \) to \( (-\infty, 0) \) with same Lipschitz constant \( L_f \). Hence, \( v = \log \sigma f \) is a function from \( \mathcal{X} \) to \( (-\infty, 0) \). Note that since \( \mathcal{X} \) is bounded
and $f$ is Lipschitz continuous from $\mathcal{X}$ to $\mathbb{R}$, we can always find some $r$ such that $v$ maps from $\mathcal{X}$ to $(-r, 0)$.

Now, we show that $v = \log \sigma f$ is Glivenko Cantelli by entropy number. Let $\mathcal{V} = \{v : v = \log(\sigma(f)), f \in \mathcal{F}\}$. In Lemma 10 we use theorem from [17] to show that $\mathcal{V}$ is Glivenko Cantelli if and only if

$$\frac{1}{m} \log N(\epsilon, \mathcal{V}, \ell_1(P_m)) \xrightarrow{p} 0,$$

for any $M > 0$, $\epsilon$, where $\mathcal{V}_M$ is the class of functions $v1\{E \leq M\}$ where $v$ ranges over $\mathcal{V}$ and $E$ is an envelope function to $\mathcal{V}$. Since we proved that $\log(\sigma(f)(x)) < 0$ for any $x$, we can choose $E = v_0(x) = 0$ as a constant function that is an envelope to $\mathcal{V}$. For any $M > 0$, therefore, $1\{E \leq M\} = 1$ trivially and $\mathcal{V}_M = \mathcal{V}$. Hence, we just need to show

$$\frac{1}{m} \log N(\epsilon, \mathcal{V}, \ell_1(P_m)) \xrightarrow{p} 0$$

In Lemma 9 we show that the entropy number of such a function is given by

$$\log N(\epsilon, \mathcal{V}, \ell_1(P_m)) \leq \left(\frac{16L.diam(\mathcal{X})}{\epsilon}\right)^{\frac{d\dim(\mathcal{X})}{\epsilon}} \log \left(\frac{4r}{\epsilon}\right),$$

and therefore is bounded and independent of the sample size $m$. Hence, $\frac{1}{m} \log N(\epsilon, \mathcal{V}, \ell_1(P_m))$ goes to 0.

**Lemma 7.** The function $f$ defined in Theorem 1 on the main paper as:

$$f(x) = \int_\mathcal{V} g(w)\psi(x, w)d\tau(w),$$

where $\psi(x, w) = \phi_\theta(x)^Tw$ and the function $\phi_\theta$ is Lipschitz continuous with Lipschitz constant $L_\phi$. Then, the function $f$ is Lipschitz continuous with some Lipschitz constant, $L_f$.

**Proof.** By the definition,

$$f(x) = \langle g(w), \psi(x, w) \rangle_{L_2(\mathcal{X})}$$

For any two points $x_1$ and $x_2$,

$$|f(x_1) - f(x_2)| = \langle g(w), \psi(x_1, w) - \psi(x_2, w) \rangle_{L_2(\mathcal{X})} \leq ||g(w)||_{L_2(\mathcal{X})}||\psi(x_1, w) - \psi(x_2, w)||_{L_2(\mathcal{X})}$$

where we used Cauchy Schwartz. Now, taking the difference in $\psi$, it can be written as

$$||\psi(x_1, w) - \psi(x_2, w)||_{L_2(\mathcal{X})} = \sqrt{\int_\mathcal{V} [\psi(x_1, w) - \psi(x_2, w)]^2d\tau(w)}$$

$$= \sqrt{\int_\mathcal{V} [\phi_\theta(x_1) - \phi_\theta(x_2)]^Tw]^2d\tau(w)}$$

$$\leq \sqrt{\int_\mathcal{V} ||\phi_\theta(x_1) - \phi_\theta(x_2)||^2||w||^2d\tau(w)}$$

where we again used Cauchy Schwartz in the last line since $[(\phi_\theta(x_1) - \phi_\theta(x_2))^Tw]$ is an inner product in $\mathbb{R}^D$ where $D$ is the dimension of $w$. Since $\phi_\theta$ is Lipschitz continuous with Lipschitz constant $L_\phi$, we have

$$||\phi_\theta(x_1) - \phi_\theta(x_2)|| \leq L_\phi ||x_1 - x_2||$$

Using this inequality in eq.74 we obtain

$$||\psi(x_1, w) - \psi(x_2, w)||_{L_2(\mathcal{X})} \leq L_\phi ||x_1 - x_2|| \sqrt{\int_\mathcal{V} ||w||^2d\tau(w)}$$

$$= L_\phi ||x_1 - x_2|| \sqrt{\text{tr}(C_w)}$$
where, $C_w$ is the uncentered covariance matrix of Gaussian distributed $w$. Plugging eq.(79) in eq.(74), we obtain

$$|f(x_1) - f(x_2)| \leq \|g(w)\|_{L_2(d\tau)} L_{\phi} \sqrt{\text{tr}(C_w)} |x_1 - x_2|$$

(80)

Since, we have that $\|g(w)\|_{L_2(d\tau)} < \infty$ (see Lemma 4), we have proved that $f$ is Lipschitz continuous with Lipschitz constant given by $L_f \leq \|g(w)\|_{L_2(d\tau)} L_{\phi} \sqrt{\text{tr}(C_w)}$. 

\[ \blacksquare \]

**Lemma 8.** The function $\log \circ \sigma$ exhibits following properties:

i) It is a concave function with its derivative always between 0 and 1

ii) If the Lipschitz constant of $f$ is $L_f$, so is the Lipschitz constant of $\log \circ \sigma \circ f$

**Proof.** i) Let us denote $u(x) = \log(\sigma(x))$. Then, we have,

$$u(x) = \log \frac{e^x}{1 + e^x} = x - \log(1 + e^x)$$

(81)

:. $u'(x) = 1 - \frac{e^x}{1 + e^x} = \frac{1}{1 + e^x}$$

(82)

:. $0 < u'(x) < 1, \quad \forall x \in (-\infty, \infty)$

(83)

which proves that the derivative is between 0 and 1. To show that $u(x)$ is concave, it is sufficient to note that its second derivative is always negative.

ii) Let us use notation $u = \log(\sigma)$, and let $f_2 = f(x_2), f_1 = f(x_1), u_2 = u(f(x_2)), u_1 = u(f(x_1))$. Since the maximum derivative of $u$ is upper bounded by 1, $u$ as a function of $f$ has Lipschitz constant 1 and therefore, we can write

$$u_2 - u_1 = u(f_2) - u(f_1) \leq f_2 - f_1 = f(x_2) - f(x_1)$$

(84)

$$\leq L_f \|x_2 - x_1\|$$

(85)

where the last inequality is because $f$ is Lipschitz continuous with Lipschitz constant $L_f$. This proves that the Lipschitz constant of $\log \circ \sigma \circ f$ is also $L_f$.

\[ \blacksquare \]

**Lemma 9.** Let $\mathcal{F}_L$ be the space of $L$-Lipschitz functions mapping the metric space $(X, \rho)$ to $[0,r]$. Let $\text{ddim}(X)$ and $\text{diam}(X)$ denote the doubling dimension and diameter of $X$ respectively. Then, i) the covering numbers of $\mathcal{F}_L$ can be estimated in terms of the covering numbers of $X$:

$$\mathcal{N}(\epsilon, \mathcal{F}_L, \|\cdot\|_{\infty}) \leq \left(\frac{4r}{\epsilon}\right)^{\mathcal{N}(\epsilon/8L, X, \|\cdot\|_{\infty})}$$

(86)

ii) the entropy number of $\mathcal{F}_L$ can be estimated as:

$$\log \mathcal{N}(\epsilon, \mathcal{F}_L, \|\cdot\|_{\infty}) \leq \left(\frac{16L \cdot \text{diam}(X)}{\epsilon}\right)^{\text{ddim}(X)} \log \left(\frac{4r}{\epsilon}\right)$$

(87)

iii) the entropy number with respect to $\ell_1(\mathbb{P}_m) = \int |f|d\mathbb{P}_m = \frac{1}{m} \sum_k |f(x_k)|$ defined with respect to the $m$ input points, is the same as (ii), i.e.

$$\log \mathcal{N}(\epsilon, \mathcal{F}_L, \ell_1(\mathbb{P}_m)) \leq \left(\frac{16L \cdot \text{diam}(X)}{\epsilon}\right)^{\text{ddim}(X)} \log \left(\frac{4r}{\epsilon}\right)$$

(88)

where $\mathbb{P}_m$ is an empirical probability measure with respect to $m$ inputs points in $X$.

**Proof.** The proof is adapted from [26] Lemma 2 and [27] Lemma 6, and modified to handle range $[0, r]$.

i) We first cover the domain $X$ by $N$ balls $U_1, U_2, \ldots, U_{|N|}$, where $N = \mathcal{N}(\epsilon/8L, X, \|\cdot\|_{\infty})$ is the covering number of $X$, $N = \{x_i \in U_1\}_{i=1}^{|N|}$ is a set of center points of $|N|$ balls and $\epsilon' = \epsilon/8L$ is the radius of the covering balls.

Now, our strategy is to construct an $\epsilon$ cover $\hat{F} = \{\hat{f}_1, \ldots, \hat{f}_{\hat{m}}\}$ for $\mathcal{F}_L$ with respect to $\|\cdot\|_{\infty}$. To do so, at every point $x_i \in N$, we choose the value of $\hat{f}(x_i)$ to be some multiple of $2L\epsilon' = \frac{\epsilon}{8}$, while
With this construction, we can show that every \( f \in \mathcal{F}_L \) is close to some \( \hat{f} \in \hat{F} \) in the sense that \( \|f - \hat{f}\|_\infty \leq \epsilon \). To show this, note the following:

\[
\begin{align*}
|f(x) - \hat{f}(x)| &\leq |f(x) - f(x_N)| + |f(x_N) - \hat{f}(x_N)| + |\hat{f}(x_N) - \hat{f}(x)| \\
&\leq L \rho(x, x_N) + \epsilon/4 + 2L \rho(x, x_N) \\
&\leq \epsilon
\end{align*}
\] (89) (90) (91)

where the inequality in eq.(90) is due to the fact that \( f \) is \( L \)-Lipschitz and \( \hat{f} \) is \( 2L \)-Lipschitz and since we have covered the input space \( \mathcal{X} \), each \( x \) is within \( \epsilon' \) of some \( x_N \). Also note that for every \( f(x_N) \) we can find \( \hat{f}(x_N) \) within some radius \( \epsilon/4 \); this is because we choose \( f(x_N) \) to be some multiple of \( 2L \epsilon' \). Finally, we need to compute the cardinality of \( \hat{F} \), i.e. \( |\hat{F}| \). For any \( x_i \in [N] \), \( \hat{f} \) can take one of the multiple of \( 2L \epsilon' \) values. Hence, there are \( r/2L \epsilon' \) such possibilities as the range is \([0, r] \).

Since there are \([N]\) such possibilities for \( x_i \), the upper bound on all possible function values \( \hat{f} \) is \((\frac{r}{2L \epsilon'})^{|N|} = (\frac{r}{2L})^{|N|}\), which proves the first statement after plugging in the value of \(|N|\).

ii) Taking logarithm of the result in i)

\[
\log \mathcal{N}(\epsilon, \mathcal{F}_L, ||\cdot||_\infty) \leq \mathcal{N}(\epsilon/8L, \mathcal{X}, ||\cdot||_\infty) \log \left( \frac{4r}{\epsilon} \right)
\] (92)

The covering number of the input space, \( \mathcal{X} \) in terms of doubling dimension, \( ddim(\mathcal{X}) \) and diameter, \( diam(\mathcal{X}) \) can be written as [30]:

\[
\mathcal{N}(\epsilon, \mathcal{X}, ||\cdot||_\infty) = \left( \frac{2diam(\mathcal{X})}{\epsilon} \right)^{ddim(\mathcal{X})}
\] (93)

Plugging this expression in eq.(92), we obtain the required expression.

iii) The result in i) is with respect to \( ||\cdot||_\infty \). In eq.(90), we showed that for any \( f \in \mathcal{F}_L \) there is some \( \hat{f} \in \hat{F} \) within a radius of \( \epsilon \) such that \( ||f - \hat{f}||_\infty \leq \epsilon \). Here, we show that this also implies that \( ||f - \hat{f}||_{\ell_1(\mathbb{P}_m)} \leq \epsilon \). We show this as follows:

\[
||f - \hat{f}||_{\ell_1(\mathbb{P}_m)} = \frac{1}{m} \sum_{k=1}^{m} |f(x_k) - \hat{f}(x_k)|
\] (94)

\[
\leq \frac{1}{m} \sum_{k=1}^{m} \epsilon = \epsilon
\] (95)

Therefore, the entropy number with respect to \( \ell_1(\mathbb{P}_m) \) metric is same as the entropy number with respect to the \( ||\cdot||_\infty \), which proves our third claim.

**Lemma 10** ([17] Theorem 3.5 ). Let \( \mathcal{V} \) be a class of measurable functions with envelope \( E \) such that \( P(E) < \infty \). Let \( \mathcal{V}_M \) be the class of functions \( v \mid E \leq M \) where \( v \) ranges over \( \mathcal{V} \). Then, \( \mathcal{V} \) is a Glivenko Cantelli class of functions, i.e. it satisfies

\[
\sup_{v \in \mathcal{V}} |\mathbb{P}_m v - P v|
\] (96)

if and only if

\[
\frac{1}{m} \log \mathcal{N}(\epsilon, \mathcal{V}_M, L_1(\mathbb{P}_m)) \overset{p}{\to} 0,
\] (97)

for every \( \epsilon > 0 \) and \( M > 0 \), where \( P v = \int v dP \) and \( \mathbb{P}_m v = \frac{1}{m} \sum_k v(x_k) \).

**D Experimental Results**

**Code:** The code will be publicly released.
D.1 Two Gaussian

D.1.1 Architecture and Implementation

RKHS Discriminator Architecture (Pytorch Code)

class RKHS_Net(nn.Module):
    def __init__(self, dim =10, mid_dim1=20, mid_dim2=20, mid_dim3=20, D=50, gamma =1, metric = 'rbf', lip=5, g_lip =5):
        super(RKHS_Net, self).__init__()
        self.gamma = torch.FloatTensor([gamma])
        self.metric = metric
        self.D = D
        self.act = nn.ReLU()
        self.lin1 = spectral_norm( nn.Linear(dim, mid_dim1), k =g_lip)
        self.lin2 = spectral_norm( nn.Linear(mid_dim1, mid_dim2), k =g_lip)
        self.lin3 = spectral_norm( nn.Linear(mid_dim2, mid_dim3), k =g_lip)
        self.lin4 = spectral_norm( nn.Linear(mid_dim3, 1), k =g_lip)
        self.g = nn.Sequential(self.lin1, self.act, self.lin2, self.act, self.lin3, self.act, self.lin4)
        self.lin_phi1 = spectral_norm(nn.Linear(2, mid_dim1), k=lip)
        self.lin_phi2 = spectral_norm(nn.Linear(mid_dim1, mid_dim2), k=lip)
        self.lin_phi3 = spectral_norm(nn.Linear(mid_dim2, mid_dim3), k=lip)
        self.lin_phi4 = spectral_norm(nn.Linear(mid_dim3, dim), k=lip)
        self.phi = nn.Sequential(self.lin_phi1, self.act, self.lin_phi2, self.act, self.lin_phi3, self.act, self.lin_phi4)
    def forward(self, y):
        x=self.phi(y)
        d = x.shape[1]
        if self.metric == 'rbf':
            w= torch.sqrt(2*torch.randn(size=(self.D,d))
            w=w.to(x.device)
            psi = ((torch.matmul(x,w.permute(1,0)))
                *(torch.sqrt(2/torch.FloatTensor([self.D])).to(x.device))
            w_a = w
            g= self.g(w_a)
            f = (psi*g.permute(1,0)).mean(1)
            g_norm = (g**2).mean()
            return f, g_norm

Simple Neural Network Discriminator Architecture (Pytorch Code)

class DNet_basic(nn.Module):
    def __init__(self, input_dim, mid_dim1, mid_dim2, output_dim, lip_constraint = False, lip = 5):
        super(DNet_basic, self).__init__()
        self.act = nn.ReLU()
Discrete approximation: Both the discriminators have stacked Fully connected layers and activation function. In the proposed RKHS discriminator, we have an additional network `self.g` which we use to approximate the continuous integral $f(x) = \int_W g(w)\psi(x,w)d\tau(w)$ with the following discrete approximation:

$$f(x) = \frac{1}{D} \sum_{k=1}^{D} g(w_k)(\phi^T w_k \sqrt{\frac{2}{D}})$$  \hspace{1cm} (98)

where $w$ is sampled from a Normal distribution with variance $\gamma$. In our experiments $D = 500$ was sufficient. Note that the Neural network discriminator is similar to $\phi^T w$, except that $w$ is not randomly sampled and there is no $g$ network.

Lipschitz constraints: To enforce Lipschitz constraints on network $g$ and $\phi$ consistent with our assumptions and theoretical results, we use spectral normalization in the RKHS discriminator while it is absent in the basic Neural network discriminator.

D.1.2 Data and Hyperparameters

Data: Since this is a toy experiment, data were generated locally using pytorch command `randn` to sample from Gaussian distribution.

Learning rate: $5 \times 10^{-3}$ (both models)
No. of samples from each distribution: 2500 (both models)
Minibatch size: 50 (both models)
$\lambda$: 0.005 (RKHS disc.)

Hyperparameter selection: (RKHS disc.) The hyperparameters like learning rate and $\lambda$ were selected by first estimating KL divergence at a mid value like 13. Then, same value was used in all experiments.

D.1.3 Computational Resources and Time

Running one experiment of KL divergence calculation takes 74 s for the basic algorithm while it takes 245 s for the proposed method in a single GeForce GTX 1080 Ti GPU with 11GB memory.

D.2 Mutual Information Estimation

D.2.1 Models, Architecture and Implementation

RKHS Discriminator Architecture (Pytorch Code)

```python
class ConcatLipFeatures(nn.Module):
    def __init__(self, input_dim, mid_dim1, mid_dim2, output_dim):
        super(ConcatLipFeatures, self).__init__()
        self.lin1 = nn.Linear(input_dim, mid_dim1)
        self.lin2 = nn.Linear(mid_dim1, mid_dim2)
        self.lin3 = nn.Linear(mid_dim2, mid_dim2)
        self.lin4 = nn.Linear(mid_dim2, output_dim)
        self.act = nn.ReLU()
        # self.sigmoid=nn.Sigmoid()

        self.phi = nn.Sequential(self.lin1,
                                 self.act,
                                 self.lin2,
                                 self.act,
                                 self.lin3,
                                 self.act,
                                 self.lin4
                               )

    def forward(self, x):
        t = self.phi(x)
        return t
```
def __init__(self, dim, hidden_dim, layers, activation, lip, gamma = 1, metric = 'rbf', D=500, mid_dim=5, g_lip=2, **extra_kwargs):
    super(ConcatCritic, self).__init__()
    self.gamma = torch.FloatTensor([gamma])
    self.metric = metric
    self.D = D
    self.act = nn.ReLU()
    self.lin1 = spectral_norm( nn.Linear(hidden_dim, mid_dim), k = g_lip)
    self.lin2 = spectral_norm( nn.Linear(mid_dim, mid_dim), k = g_lip)
    self.lin3 = spectral_norm( nn.Linear(mid_dim, mid_dim), k = g_lip)
    self.lin4 = spectral_norm( nn.Linear(mid_dim, 1), k = g_lip)
    self.g = nn.Sequential(self.lin1, self.act, self.lin2, self.act, self.lin3, self.act, self.lin4)

    self.rkhs_layer = feature_perceptron(dim * 2, hidden_dim, 1, layers, activation, lip)

    def forward(self, x, y):
        batch_size = x.size(0)
        x_tiled = torch.stack([x] * batch_size, dim=0)
        y_tiled = torch.stack([y] * batch_size, dim=1)
        xy_pairs = torch.reshape(torch.cat((x_tiled, y_tiled), dim=2), [batch_size * batch_size, -1])
        phi = self.rkhs_layer(xy_pairs)
        d = phi.shape[1]
        if self.metric == 'rbf':
            w = torch.sqrt(2 * self.gamma) * torch.randn(size=(self.D, d)).to(x.device)
            psi = ((torch.matmul(phi, w.permute(1, 0))) * (torch.sqrt(2 / torch.FloatTensor([self.D])).to(x.device)))
            w_a = w
            g = self.g(w_a)
            f = (psi * g.permute(1, 0)).mean(1)
            g_norm = (g ** 2).mean()
            return f, g_norm

Simple Neural Network Discriminator Architecture (Pytorch Code)

class ConcatCritic(nn.Module):
    def __init__(self, dim, hidden_dim, layers, activation, **extra_kwargs):
        super(ConcatCritic, self).__init__()
        self._f = mlp(dim * 2, hidden_dim, 1, layers, activation)

    def forward(self, x, y):
        batch_size = x.size(0)
        x_tiled = torch.stack([x] * batch_size, dim=0)
        y_tiled = torch.stack([y] * batch_size, dim=1)
        xy_pairs = torch.reshape(torch.cat((x_tiled, y_tiled), dim=2), [batch_size * batch_size, -1])
        scores = self._f(xy_pairs)
return torch.reshape(scores, [batch_size, batch_size]).t()

Similar to the previous experiment, the RKHS discriminator and the Neural network discriminator are similar in core design. The main difference lies in that the RKHS discriminator has this inner product construction same as eq. (1) in previous subsection. To achieve this construction, the RKHS discriminator an additional network, self.g and enforces Lipschitz constraint through spectral normalization, which are absent in simple Neural network discriminator.

D.2.2 Data and Hyperparameters

Data: The experimental setup and data generation follow https://github.com/ermongroup/smile-mi-estimator.

Common for all methods
- batch size: 64
- no. of layers: 2
- hidden dim: 256
- no. of iterations: 40000
- learning rate: $5 \times 10^{-4}$

Specific to the proposed method
- $\gamma$: 5
- Lipschitz constant enforced, $L_\phi$ (layer wise): 5
- Lipschitz constant enforced, $L_g$ (layer wise): 5

D.2.3 Computational Resources and Time

GPU: GeForce RTX 2080 Ti 11 GB

Below, we report time taken by each method to complete an experiment to obtain mutual information between two 20-d Gaussian distributed random variables using 40,000 samples from each distribution and mutual information increasing stepwise.

Table 1: Time taken to complete one experiment

|      | CPC | NWJ | SMILE | Ours (RKHS disc.) |
|------|-----|-----|-------|-------------------|
| Time | 52 s| 48 s| 52 s  | 63 s              |

D.2.4 Existing Assets

We used the code from the repo https://github.com/ermongroup/smile-mi-estimator to generate data as well as run baseline mutual information methods. This code corresponds to the Song et al. [9].

D.3 Adversarial Variational Bayes

D.3.1 Models, Architecture and Implementation

RKHS Discriminator Architecture (Pytorch Code)

```python
class Discriminator_RKHS(nn.Module):
    def __init__(self, x_dim, h_dim, z_dim, lip = 5, g_lip = 5, dim = 10, mid_dim1 = 20, mid_dim2 = 20, mid_dim3 = 20, D=100, gamma =1, metric = 'rbf'):
        super(Discriminator_RKHS, self).__init__()
        self.metric = metric
        self.gamma = torch.FloatTensor([gamma])
        self.D = D
        self.phi = nn.Sequential(
            nn.Linear(x_dim + z_dim, h_dim), k = lip),
            n.LeakyReLU(),
            spectral_norm(nn.Linear(h_dim, h_dim), k = lip),
```
Simple Neural Network Discriminator Architecture (Pytorch Code)

class Discriminator_simple(nn.Module):
    def __init__(self, x_dim, h_dim, z_dim):
        super(Discriminator_simple, self).__init__()
        self.net = nn.Sequential(
            nn.Linear(x_dim + z_dim, h_dim),
            nn.LeakyReLU(),
            nn.Linear(h_dim, h_dim),
            nn.LeakyReLU(),
            nn.Linear(h_dim, h_dim),
            nn.LeakyReLU(),
            nn.Linear(h_dim, h_dim),
            nn.LeakyReLU(),
            nn.Linear(h_dim, int(h_dim/4)),
            nn.LeakyReLU(),
            nn.Linear(int(h_dim/4), 1),

def weight_init(self, mean, std):
    for m in self._modules:
        normal_init(self._modules[m], mean, std)

def forward(self, y, z):
    y = y.view(y.shape[0], -1)
    y = torch.cat([y, z], 1)
    x = self.phi(y)
    d = x.shape[1]
    if self.metric == 'rbf':
        w = torch.sqrt(2 * self.gamma) * torch.randn(size=(self.D, d))
        w = w.to(x.device)
        psi = ((torch.matmul(x, w.permute(1, 0)))) * (torch.sqrt(2 /
            torch.FloatTensor([self.D])).to(x.device))
        w_a = w
        g = self.g(w_a)
        f = (psi * g.permute(1, 0)).mean(1)
        g_norm = (g ** 2).mean()
        return f, g_norm
```python
def weight_init(self, mean, std):
    for m in self._modules:
        normal_init(self._modules[m], mean, std)

def forward(self, x, z):
    x = x.view(x.shape[0], -1)
    x = torch.cat([x, z], 1)
    out = self.net(x)
    # x = x + torch.sum(z ** 2, 1)
    return out
```

D.3.2 Data and Hyperparameters

Data: Standard MNIST dataset is used.

Learning rate: \(10^{-3}\) (both models)
Minibatch size: 1024 (both models)
Hidden dim of encoder/decoder: 800 (both)
Hidden dim discriminator: 1024 (both)
\(\lambda\) : 1 (RKHS disc.)

D.3.3 Computational Resources and Time

GPU: GeForce GTX 1080 Ti 11GB
Time taken to train MNIST for 1000 epochs using AVB with simple Neural net discriminator: 11.3 hrs
Time taken to train MNIST for 1000 epochs using AVB with RKHS discriminator: 14.7 hrs

D.3.4 Existing Assets

We followed the official implementation of Adversarial Variational Bayes [8] at https://github.com/LMescheder/AdversarialVariationalBayes

E Societal Impacts

We discuss possible negative impacts in two categories: 1) Impact of theoretical contribution, 2) Impact of applications

**Societal Impact of theoretical contribution:** The main theoretical contribution of the paper is its connection between reliable/stable estimation and complexity analysis of the discriminator function space. In its general form, this contribution does not, by itself, pose any negative societal impact. Rather, it is about stabilizing algorithms. So, it contributes towards more robust and stable algorithms, and may help in developing more secure applications. We do not foresee any negative societal impacts in safety and security of human beings and automatic systems, human rights, human livelihood or economic security, environment. We do not see it causing theft, harassment, fraud, bias or discrimination.

**Societal Impact of possible applications:** As demonstrated in the experiment section, this work can be applied to information theoretic applications that require mutual information or KL divergence estimation. For example, it has been used in generative modeling like variational autoencoder, variational Bayes or in stabilizing generative adversarial networks (GANs). These generative modeling techniques are, by themselves, quite general and can have numerous applications, including the ones with negative impacts. By helping in accurate estimation of KL divergence and by providing theoretical analysis, this work is contributing to develop stronger generative models and by extension could be indirectly helping in their negative uses. In that aspect, we appeal everyone using the algorithms and ideas in this paper to be thoughtful and responsible in their use.