ABSTRACT

Several recent works in communication systems have proposed to leverage the power of neural networks in the design of encoders and decoders. In this approach, these blocks can be tailored to maximize the transmission rate based on aggregated samples from the channel. Motivated by the fact that, in many communication schemes, the achievable transmission rate is determined by a conditional mutual information, this paper focuses on neural-based estimators for this information-theoretic quantity. Our results are based on variational bounds for the KL-divergence and, in contrast to some previous works, we provide a mathematically rigorous lower bound. However, additional challenges with respect to the unconditional mutual information emerge due to the presence of a conditional density function; this is also addressed here.

Index Terms— channel capacity, conditional mutual information, variational bounds, neural networks

1. INTRODUCTION

Although originally conceived to address communication problems, information-theoretic measures have been insightful in many fields including statistics, signal processing, and even neuroscience. Entropy, KL-divergence, and mutual information (MI) are extensively used to explain the behavior and relation among random variables. For example, MI and its extensions are used to characterize the capacity of communication channels [1] as well as define notions of causality [2, 3]. Information-theoretic quantities have also made their way into machine learning and deep neural networks [4]. They have been adopted to regularize optimizations in neural networks [5] and Markov decision processes [6], or to express the flow of information in layers of a deep network [7]. In a generative adversarial network (GAN), in which a neural network is optimized to perform towards the best-trained adversary, the relative entropy plays an eminent role [8, 9].

On the other hand, neural networks have also been applied in communication setups as part of the encoder/decoder blocks [10, 11, 12]. Learning the end-to-end communication system is challenging though, and requires the knowledge of the channel model, which it is not available in many applications. One solution to this problem is to train a GAN model to mimic the channel, which can later be used to learn the whole system [13, 14]. Alternatively, one can design encoders and optimize them to achieve the maximum rate (capacity), which is characterized by the MI. In [15], the authors exploit a neural network estimator of the mutual information proposed in [16] to optimize their encoders. Although estimating the MI has been studied extensively (see e.g., [17, 18]), the capacity in many communication setups (such as the relay channel, channels with random state, wiretap channels) is described by the conditional mutual information (CMI), which requires specialized estimators. Extending the existing estimators of MI for this purpose is not trivial and is the main focus of this paper. Motivated by [15], we investigate estimators using artificial neural networks.

The main challenges in estimating the CMI stem from empirically computing the conditional density function and from the curse of dimensionality. The latter is, in fact, a common problem in many data-driven estimators for MI and CMI. A conventional estimator in the literature for MI is based on the \(k\)-nearest neighbors (\(k\)-NN) method [19], which has been extensively studied [20] and extended to estimate CMI [21, 22, 23]. In a recent work, the authors of [16] propose a new approach to estimate the MI using a neural network, which is based on the Donsker–Varadhan representation of the KL-divergence [24]. Improvements are shown in the performance of estimating the MI between high-dimensional variables compared to the \(k\)-NN method. Several other works also take advantage of variational bounds [25] to estimate the MI and show similar improvements [26, 27].

For estimating the CMI, the authors of [28] introduce a neural network classifier to categorize the density of the input into two classes (joint and product); then they show that by training such classifier, they can optimize a variational bound for the relative entropy and correspondingly for the MI and the CMI. Furthermore, they suggest the use of a GAN model, a variational autoencoder, and \(k\)-NN to generate or select samples with the appropriate conditional density.

Although the trained classifier proposed in [28] asymptotically converges to the optimal function for the variational
bound, a relatively high variance can be observed in the final output. Consequently, the final estimation is an average over several Monte Carlo trials. However, the variational bound used in [28] contains non-linearities which results in a biased estimation when taking a Monte Carlo average. A similar problem is pointed out in [27] where the authors suggest a looser but linear variational bound. In this paper, we take advantage of the classifier technique applied to a linearized variational bound to avoid the bias problem. For simplicity, the $k$-NN method is used to collect samples from the conditional density. In Section 2 the variational bounds are explained and we shed light on the Monte Carlo bias problem. Afterwards, the proposed technique to train the classifier and estimate the CMI is stated in Section 3. Then, we investigate the problem of estimating the secrecy capacity of the degraded wiretap channel characterized by the CMI. Finally the paper is concluded in Section 4.

2. PRELIMINARIES

For random variables $X, Y, Z$ jointly distributed according to $p(x, y, z)$, the CMI is defined as:

$$I(X; Y | Z) = D_{KL}(p(x, y, z) \parallel p(y, z)p(x | z)),$$

(1)

where $D_{KL}(p \parallel q)$ is the KL-divergence between the probability density functions (pdfs) $p(u)$ and $q(u)$, $u \in \mathbb{R}$,

$$D_{KL}(p \parallel q) = \int p(u) \log \frac{p(u)}{q(u)} du.$$

(2)

The CMI characterizes the capacity of communication systems such as channels with random states, network communication models like the relay channel or the degraded wiretap channel (DWTC)[1]. For example, in the DWTC (see Fig. 1), the secrecy capacity is:

$$C_s = \max_{p(x)} I(X; Y | Z).$$

(3)

By similar steps as in [25], we can bound (1) from below:

$$I(X; Y | Z) \geq E_{p(x, y, z)} \left[ \log \frac{q(x | y, z)}{p(x | z)} \right],$$

(4)

where $q(x | y, z)$ is any arbitrary pdf; the last step holds true since the relative entropy is non-negative. The lower bound in (4) is tight if the conditional density functions $p(x | y, z)$ and $q(x | y, z)$ are equal. As discussed in [27], by choosing an energy-based density, one can obtain lower bounds for the CMI as stated in the following proposition.

**Proposition 1.** For any function $f : \mathcal{X} \times \mathcal{Y} \times \mathcal{Z} \to \mathbb{R}$, let $M(y, z) = E_{p(x)} \left[ \exp f(x, y, z) \right]$, then the following bound holds and is tight when $f(x, y, z) = \log p(y | x, z) + c(y, z)$:

$$I(X; Y | Z) \geq E_{p(x, y, z)} \left[ f(x, y, z) \right] - E_{p(y, z)} \left[ \log M(y, z) \right].$$

(5)

**Proof.** Choosing $q(x | y, z) := \frac{p(x | y, z) \exp f(x, y, z)}{M(y, z)}$ and substituting in (4) yields the desired bound. \square

It is worth noting that computing the optimal $f(x, y, z)$ is non-trivial since we may not have access to the joint pdf. Using Proposition 1 and Jensen’s inequality, a variant of the Donsker–Varadhan bound [24] can be obtained as follows:

$$I(X; Y | Z) \geq E_{p(x, y, z)} \left[ f(x, y, z) \right] - \log E_{p(y, z)} \left[ \exp f(x, y, z) \right].$$

(6)

Hereafter let the r.h.s. of (6) be denoted as $I_{DV}$. The bound is tight when $f(x, y, z) = \log \frac{p(x | y, z)}{p(x | z)} + c$.

In order to estimate $I_{DV}$ from samples, an empirical average may be taken with respect to $p(x, y, z)$ and $p(x | z)p(y, z)$. Let $B^b_{\text{joint}}$ and $B^b_{\text{prod}}$ be a random batch of $b$ triples $(x, y, z)$ sampled respectively from $p(x, y, z)$ and $p(x | z)p(y, z)$; then the estimated $I_{DV}$ for an arbitrary choice of $f(x, y, z)$ is:

$$\hat{I}_{DV} = \frac{1}{b} \sum_{(x, y, z) \in B^b_{\text{joint}}} f(x, y, z) - \log \frac{1}{b} \sum_{(x, y, z) \in B^b_{\text{prod}}} \exp f(x, y, z).$$

(7)

Since the outcomes of the previous estimator exhibit a relatively high variance (27)28,29, the authors of [28] averaged the estimated results over several trials. However, due to the concavity of the logarithm in the second term of $I_{DV}$, a Monte Carlo average of different instances of $I_{DV}$ creates an upper bound for $I_{DV}$, while $I_{DV}$ is itself a lower bound of the CMI. This issue can be resolved by taking a looser bound where the log term is linearized. A similar bound is obtained by Nguyen, Wainwright, and Jordan 30, also adopted in [16][28] to estimate the MI and which was denoted $f$-MINE (since it corresponds to a variational representation for the divergence). The corresponding bound for the CMI is:

$$I(X; Y | Z) \geq E_{p(x, y, z)} \left[ f(x, y, z) \right] - e^{-1} E_{p(x | z)p(y, z)} \left[ \exp f(x, y, z) \right],$$

(8)

where we use $\log(u) \leq e^{-1} u$ in [6]. In this paper, let $I_{NWJ}$ refer to the lower bound (8). The bound is tight for $f(x, y, z) = \log \frac{p(x | y, z)}{p(x | z)} + c$. 

![Fig. 1: Degraded wiretap channel.](image)
1 + \log \frac{p(x|y, z)}{p(x|z)}$, while a Monte Carlo average of several instances of the estimator $\hat{I}_{NWJ}$ is unbiased and, consequently, justified for estimating a lower bound on the CMI.

Although the optimal choice for $f(x, y, z)$ is known, since the true joint density is unknown, it is non-trivial to compute. Several approaches have been proposed to estimate $I_{NWJ}$ for MI and CMI including \cite{16, 22, 28}. In \cite{16}, the searching space is restricted to functions generated via a neural network; then using minibatch gradient descent, the r.h.s. of (8) is optimized. Even though training the network can be unstable \cite{22}, their method is shown to scale better with dimension than the k-NN estimator for mutual information in \cite{19}. Alternatively, \cite{27} discusses estimators for log density ratio as input and corresponding output $\omega$, where the objective is to classify the samples. Using a sigmoid function $\sigma(\omega)$, one can map the $\omega$ to a real value in $(0, 1)$. Let $c$ be the classifier’s decision and assume cross-entropy loss defined as

$$L(\theta) = -\frac{1}{n} \sum_{i=1}^{n} c_i \log(\sigma(\omega)) + (1 - c_i) \log(1 - \sigma(\omega_i))$$  \hspace{1cm} (9)$$

to be minimized; it is conventional to denote $\sigma(\omega)$ as $\Pr(c = 1|x, y, z)$. With a sufficient number of samples and by the central limit theorem, the loss function converges to its expected value. Thus, for a sufficiently trained network, the output $\omega$ is close to the optimal $\omega^*$ which verifies that:

$$\lambda(\omega^*) := \frac{\sigma(\omega^*)}{1 - \sigma(\omega^*)} = \frac{p(x, y, z)}{p(x|z)p(y, z)}.$$  \hspace{1cm} (10)$$

In conclusion, by minimizing the cross-entropy loss, the trained network generates the output $\omega$ which determines the density ratio between the pdf’s for a particular triple $(x, y, z)$.

3.3. Lower bound on $I(X; Y | Z)$

We choose to estimate the CMI with $I_{NWJ}$ since it is unbiased and shown to be tight. We train a neural-network–based classifier as previously described and compute (10), this allows us to obtain the optimal $f^*(\cdot)$ for \cite{3}, i.e.,

$$f^*(x, y, z) = 1 + \log \lambda(\omega^*).$$  \hspace{1cm} (11)$$

Hence the empirical estimation is computed as:

$$\hat{I}_{NWJ}^b = 1 + \frac{1}{b} \sum b_{\text{joint}} \log \lambda(\omega^*) - \frac{1}{b} \sum b_{\text{prod}} \lambda(\omega^*).$$  \hspace{1cm} (12)$$

The steps of the estimation are stated in Algorithm 1

3.4. Numerical results

Wiretap channel As motivated in Section 1, estimators for CMI can be adopted to compute the capacity in communication systems and optimize encoders accordingly. One example is the DWTC (Fig. 1) where a source is transmitting a
message to a legitimate receiver while keeping it secret from an eavesdropper who has access to a degraded signal. The secrecy capacity \([13]\) can be estimated if samples of \((x, y, z)\) are available. Consider the channels \(p(y|x)\) and \(p(z|y)\) to have additive Gaussian noise with variance \(\sigma_1^2\) and \(\sigma_2^2\), respectively, then the model simplifies as shown in Fig. 2. So for any input \(X\) such that \(\text{Var}[X] = P\), \(I(X; Y|Z)\) can be computed as:

\[
I(X; Y|Z) = I(X; Y) - I(X; Z) 
\leq \frac{1}{2} \log \left( 1 + \frac{P}{\sigma_1^2} \right) - \frac{1}{2} \log \left( 1 + \frac{P}{\sigma_1^2 + \sigma_2^2} \right), \tag{13}
\]

with equality when \(X \sim \mathcal{N}(0, P)\). For our estimation, we consider \(\sigma_1^2 = 1\) and the input \(X\) to be zero-mean Gaussian with variance \(P = 100\); we collect \(n = 10^4\) samples of \((x, y, z)\) according to the described model and create batches of size \(b = n/2\). The neural network in our experiment has two layers with 64 hidden ReLU activation units, and we use Adam optimizer with a learning rate \(10^{-3}\) and 100 epochs. Final estimations are the averages of \(T = 20\) Monte Carlo trials.

The estimated CMI is depicted with respect to \(\sigma_2\) in Fig. 3 and for different choices of the number of neighbors \(k\). For \(\sigma_2 = 0\), i.e., the eavesdropper has access to the same signal as the legitimate receiver, the secrecy capacity is zero. It can be observed that increasing \(k\) results in a better estimation, since \(k\)-NN density estimator is shown to be consistent asymptotically when \(k \rightarrow \infty\) and \(n/k \rightarrow \infty\).

### Monte Carlo bias

To give some insights into the discussion on Section 2, we compare the estimators \(\hat{I}_{DV}\) and \(\hat{I}_{NWJ}\) for the previously defined DWTC (fixing \(\sigma_2 = 4\)) in Fig. 4. The classifier is trained with \(n = 10^4\) samples, batch size \(b = n/2\), and \(k = 100\) neighbors; to compute the lower bound, the batches \(B_{j, \text{test}}^b\) and \(B_{\text{prod}, \text{test}}^b\) are chosen with size \(b'\) and the results are averaged over \(T = 20\) Monte Carlo trials. This procedure is repeated 10 times to produce the boxplots.

It can be observed that, for small values of \(b'\), averaging the lower bound \([7]\) over trials actually yields an overestimation of the true CMI far more often than with \([12]\). This is a joint effect of the Monte Carlo bias and the small sample size—the latter affecting both estimators. Although not shown here, by increasing \(T\), the variance of the estimators is reduced, but the mean of \(\hat{I}_{DV}\) still remains above the true CMI for small \(b'\). This justifies our decision in using \(\hat{I}_{NWJ}\).

### 4. CONCLUSION

In this paper, we investigated the problem of estimating the conditional mutual information using a neural network. This was motivated by its application in learning encoders in communication systems. Since the conventional methods to estimate information-theoretic quantities do not scale well with dimension, recent works have proposed to estimate them utilizing neural networks. Although not shown in this work due to lack of space, our estimator also exhibits a better scaling with dimension than non–neural-based estimators.

Challenges of the extensions from estimators of mutual information have been discussed. Additionally, we argued on the advantages of our method in terms of estimation bias and showed the performance in estimating the secrecy transmission rate in a degraded wiretap channel. As a future direction, this method can be applied to other communication schemes and coupled with an optimizer for encoders.
5. REFERENCES

[1] A. El Gamal and Y.-H. Kim, *Network information theory*. Cambridge University Press, 2011.

[2] C. J. Quinn, T. P. Coleman, N. Kiyavash, and N. G. Hatsopoulos, “Estimating the directed information to infer causal relationships in ensemble neural spike train recordings,” *J. Comput. Neurosci.*, vol. 30, no. 1, pp. 17–44, Feb. 2011.

[3] S. Molavipour, G. Bassi, and M. Skoglund, “Testing for directed information graphs,” in 2017 55th Annual Allerton Conf. on Comm., Control, Comput. (Allerton), Oct. 2017, pp. 212–219.

[4] N. Tishby, F. C. Pereira, and W. Bialek, “The information bottleneck method,” *arXiv:physics/0004057*, Apr. 2000.

[5] R. D. Hjelm, A. Fedorov, S. Lavoie-Marchildon, K. Grewal, P. Bachman, A. Trischler, and Y. Bengio, “Learning deep representations by mutual information estimation and maximization,” *arXiv:1808.06670*, Aug. 2018.

[6] T. Tanaka, H. Sandberg, and M. Skoglund, “Transfer-entropy-regularized markov decision processes,” *arXiv:1708.09096*, Aug. 2017.

[7] M. Gabrić, A. Manoel, C. Luneau, N. Macris, F. Krzakala, L. Zdeborová et al., “Entropy and mutual information in models of deep neural networks,” in *Adv. Neural. Inf. Process. Syst.*, 2018, pp. 1821–1831.

[8] I. Goodfellow, J. Pouget-Abadie, M. Mirza, B. Xu, D. Warde-Farley, S. Ozair, A. Courville, and Y. Bengio, “Generative adversarial nets,” in *Adv. Neural. Inf. Process. Syst.*, 2014, pp. 2672–2680.

[9] S. Nowozin, B. Cseke, and R. Tomioka, “F-GAN: Training generative neural samplers using variational divergence minimization,” in *Adv. Neural. Inf. Process. Syst.*, 2016, pp. 271–279.

[10] T. O’Shea and J. Hoydis, “An introduction to deep learning for the physical layer,” *IEEE Trans. on Cogn. Commun. Netw.*, vol. 3, no. 4, pp. 563–575, Dec. 2017.

[11] S. Dörner, S. Cammerer, J. Hoydis, and S. ten Brink, “Deep learning based communication over the air,” *IEEE J. Sel. Topics Signal Process.*, vol. 12, no. 1, pp. 132–143, Feb. 2018.

[12] R. Fritschek, R. F. Schaefer, and G. Wunder, “Deep learning for the Gaussian wiretap channel,” in 2019 *IEEE Int. Conf. Comm. (ICC)*, May 2019, pp. 1–6.

[13] H. Ye, G. Y. Li, B.-H. F. Juang, and K. Sivanesan, “Channel agnostic end-to-end learning based communication systems with conditional GAN,” in 2018 *IEEE Globecom Workshops*, Dec. 2018, pp. 1–5.

[14] T. J. O’Shea, T. Roy, N. West, and B. C. Hibburn, “Physical layer communications system design over-the-air using adversarial networks,” in 2018 *26th European Signal Process. Conf. (EUSIPCO)*, Sep. 2018, pp. 529–532.

[15] R. Fritschek, R. F. Schaefer, and G. Wunder, “Deep learning for channel coding via neural mutual information estimation,” *arXiv:1903.02065*, Mar. 2019.

[16] M. I. Belghazi, A. Baratin, S. Rajeshwar, S. Ozair, Y. Bengio, A. Courville, and D. Hjelm, “MINE: Mutual Information Neural Estimation,” in 35th *Int. Conf. Mach. Learn. (ICML)*, Jul. 2018, pp. 531–540.

[17] Q. Wang, S. R. Kulkarni, and S. Verdú, “Universal estimation of information measures for analog sources,” *Foundations and Trends® in Communications and Information Theory*, vol. 5, no. 3, pp. 265–353, 2009.

[18] L. Paninski, “Estimation of entropy and mutual information,” *Neural Computation*, vol. 15, no. 6, pp. 1191–1253, Jun. 2003.

[19] A. Kraskov, H. Stögbauer, and P. Grassberger, “Estimating mutual information,” *Physical Review E*, vol. 69, no. 6, p. 066138, Jun. 2004.

[20] W. Gao, S. Oh, and P. Viswanath, “Demystifying fixed k-nearest neighbor information estimators,” *IEEE Trans. Inf. Theory*, vol. 64, no. 8, pp. 5629–5661, Aug. 2018.

[21] J. Runge, “Conditional independence testing based on a nearest-neighbor estimator of conditional mutual information,” *arXiv:1709.01447*, Sep. 2017.

[22] M. Vejmelka and M. Paluš, “Inferring the directionality of coupling with conditional mutual information,” *Physical Review E*, vol. 77, no. 2, p. 026214, Feb. 2008.

[23] S. Frenzel and B. Pompe, “Partial mutual information for coupling analysis of multivariate time series,” *Phys. Rev. Lett.*, vol. 99, no. 20, p. 204101, Nov. 2007.

[24] M. D. Donsker and S. S. Varadhan, “Asymptotic evaluation of certain Markov process expectations for large time. IV,” *Communications on Pure and Applied Mathematics*, vol. 36, no. 2, pp. 183–212, Mar. 1983.

[25] D. Barber and F. V. Agakov, “The IM algorithm: a variational approach to information maximization,” in *Adv. Neural. Inf. Process. Syst.*, 2003, pp. 201–208.

[26] A. van den Oord, Y. Li, and O. Vinyals, “Representation learning with contrastive predictive coding,” *arXiv:1807.03748*, Jul. 2018.

[27] B. Poole, S. Ozair, A. van den Oord, A. A. Alemi, and O. Vinyals, “Representation learning with contrastive predictive coding,” *arXiv:1807.03748*, Jul. 2018.

[28] S. Mukherjee, H. Asnani, and S. Kannan, “CCMI: Classifier based Conditional Mutual Information Estimation,” *arXiv:1906.01824*, Jun. 2019.

[29] D. Barber and F. V. Agakov, “The IM algorithm: a variational approach to information maximization,” in *Adv. Neural. Inf. Process. Syst.*, 2003, pp. 201–208.

[30] A. van den Oord, Y. Li, and O. Vinyals, “Representation learning with contrastive predictive coding,” *arXiv:1807.03748*, Jul. 2018.

[31] B. Poole, S. Ozair, A. van den Oord, A. A. Alemi, and G. Tucker, “On variational lower bounds of mutual information,” in *NeurIPS Workshop on Bayesian Deep Learning*, Dec. 2018.

[32] S. Mukherjee, H. Asnani, and S. Kannan, “CCMI: Classifier based Conditional Mutual Information Estimation,” *arXiv:1906.01824*, Jun. 2019.

[33] D. McAllester and K. Statos, “Formal limitations on the measurement of mutual information,” *arXiv:1811.04251*, Nov. 2018.