C-MI-GAN: Estimation of Conditional Mutual Information using MinMax formulation

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Abstract

Estimation of information theoretic quantities such as mutual information and its conditional variant has drawn interest in recent times owing to their multifaceted applications. Newly proposed neural estimators for these quantities have overcome severe drawbacks of classical $k$NN-based estimators in high dimensions. In this work, we focus on conditional mutual information (CMI) estimation by utilizing its formulation as a minmax optimization problem. Such a formulation leads to a joint training procedure similar to that of generative adversarial networks. We find that our proposed estimator provides better estimates than the existing approaches on a variety of simulated data sets comprising linear and non-linear relations between variables. As an application of CMI estimation, we deploy our estimator for conditional independence (CI) testing on real data and obtain better results than state-of-the-art CI testers.

1 INTRODUCTION

Quantifying the dependence between random variables is a quintessential problem in data science \cite{renyi1959, joe1989, fukumizu2008}. A widely used measure across statistics is the Pearson correlation and partial correlation. Unfortunately, these measures can capture and quantify only linear relation between variables and do not extend to non-linear cases. The field of information theory \cite{cover2012} gave rise to multiple functionals of data density that capture the dependence between variables even in non-linear cases. Two noteworthy quantities of widespread interest are the mutual information (MI) and conditional mutual information (CMI).

Our focus in this work is the estimation of CMI, which provides the degree of dependence between two pairs of random variables $X$ and $Y$ given a third variable $Z$. CMI provides a strong theoretical guarantee that $I(X;Y|Z) = 0 \iff X \perp Y | Z$. So, one motivation for estimation of CMI is its use in conditional independence (CI) testing and detecting causal associations. \cite{runge2018} built a CI tester using $k$NN based CMI estimator coupled with a local permutation scheme. The CI tester was found to be better calibrated than the kernel tests. CMI was used for detecting and quantifying causal associations in spike trains data from neuron pairs \cite{li2011}. In \cite{runge2019}, the authors demonstrate how CMI estimator can be combined with a causal recovery algorithm for identifying causal links in a network of variables.

Apart from its use in CI testers, CMI has found diverse applications in feature selection, communication, network inference and image processing. Selecting features iteratively so that the information is maximized given already selected features was the basis for Conditional Mutual Information Maximization (CMI) criterion in \cite{fleuret2004}. This principle was applied by \cite{wang2004} for text categorization, where the number of features are quite large. Efficient methods for CMI based feature selection involving more than one conditioning variable was developed by \cite{shishkin2016}. In the field of communications, \cite{yang2007} maximized CMI between target and reflected waveforms for optimal radar waveform design. For learning gene regulatory network, in \cite{zhang2012} CMI was used as a measure of dependence between genes. A similar approach was adapted for protein modulation in \cite{giorgi2014}. Finally, \cite{loeckx2009} used CMI as a similarity metric for non-rigid image registration. Given the widespread use of CMI as a measure of conditional dependence, there is a pressing need to accurately estimate this quantity, which we seek to achieve in this paper.
2 RELATED WORK

One of the simplest methods for estimating MI (or CMI) could be based on the binning of the continuous random variables, estimating probability densities from the bin frequencies and plugging it in the expression for MI (or CMI). Kernel methods, on the other hand, estimate the densities using suitable kernels. The most widely used estimator of MI, the KSG estimator, is based on $k$ nearest neighbor statistics (Kruskova et al. 2004) and has been shown to outperform binning or kernel-based methods. KSG is based on expressing MI in terms of entropy

$$I(X;Y) = H(X) + H(Y) - H(X;Y) \quad (1)$$

The entropy estimation follows from $H(X) = -N^{-1} \sum \log \mu(x_i)$ (Kozachenko and Leonenko 1987). Distance of the $k$ nearest neighbors of point $x_i$ is used to approximate the density $\mu(x_i)$. The KSG estimator does not estimate each entropy term independently, but accounts for the appropriate bias correction terms in the overall estimation. It ensures that an adaptive $k$ is used for distances in marginal spaces $X$ and $Y$ and for the joint space $(X,Y)$. Several later works studied the theoretical properties of the KSG estimator and sought to improve its accuracy (Gao et al. 2015, 2016, 2018; Poczos and Schneider 2012) since CMI can be expressed as a difference of two MI estimates, $I(X;Y|Z) = I(X;Y) - I(X;Z)$, the KSG estimator could be used for CMI as well. Even though the KSG estimator enjoys the favorable property of consistency, its performance in finite sample regimes suffers from the curse of dimensionality. In fact, the KSG estimator requires exponentially many samples for accurate estimation of MI (Gao et al. 2015). This limits its applicability in high dimensions with few samples.

Deviating from the $k$NN-based estimation paradigm, Belghazi et al. (2018) proposed a neural estimation of MI (referred to as MINE). This estimator is built on optimizing dual representations of the KL divergence, namely the Donsker-Varadhan (Donsker and Varadhan 1975) and the f-divergence representation (Nguyen et al. 2018). MINE is strongly consistent and scales well with dimensionality and sample size. However, recent works found the estimates from MINE to have high variance (Poole et al. 2019; Oord et al. 2018) and the optimization to be unstable in high dimensions (Mukherjee et al. 2019). To counter these issues, variance reduction techniques were explored in Song and Ermon (2020).

While for the estimation of MI we need to perform the trivial task of drawing samples from the marginal distribution, CMI estimation adds another layer of intricacy to the problem. For the above approaches to work for CMI, one needs to obtain samples from the conditional distribution. In Mukherjee et al. (2019), the authors separate the problem of estimating CMI into two stages by first estimating the conditional distribution and then using a divergence estimator. However, being coupled with an initial conditional distribution sampler, this technique is limited by the goodness of the conditional samplers and thus may be sub-optimal. Even when CMI is obtained as a difference of two separate MI estimates (CCMI estimator in Mukherjee et al. 2019), there is no guarantee that the bias values would be same from both MI terms, thereby leading to incorrect estimates. Based on these observations, in this paper, we attempt to estimate CMI using a joint training procedure involving a min-max formulation devoid of explicit conditional sampling.

The main contributions of our paper are as follows:

- We formulate CMI as a minimax optimization problem and illustrate how it can be estimated from joint training. The estimation process has similar flavor to adversarial training (Goodfellow et al. 2014) and so the term C-MI-GAN (read ”See-Me-GAN”) is coined for the estimator.
- We empirically show that estimates from C-MI-GAN are closer to the ground truth as compared to the estimates of other CMI estimators.
- We apply our estimator for conditional independence testing on a real flow-cytometry dataset and obtain better results than state-of-the-art CI Testers.

3 PROPOSED METHODOLOGY

Information Theoretic Quantities. Let $X$, $Y$ and $Z$ be three continuous random variables that admit densities. The mutual information between two random variables $X$ and $Y$ measures the amount of dependence between them and is defined as

$$I(X;Y) = \int \int P_{XY}(x,y) \log \frac{P_{XY}(x,y)}{P_X(x)P_Y(y)} dx dy \quad (2)$$

It can also be expressed in terms of the entropies as follows:

$$I(X;Y) = H(X) - H(X|Y) = H(Y) - H(Y|X) \quad (3)$$

Here $H(X)$ is the entropy of $X$ and is given by $H(X) = \int p(x) \log p(x) dx$. The above expression provides the intuitive explanation of how the information content changes when the random variable is alone versus when another random variable is given.

\footnote{More precisely, differential entropy in case of continuous random variables.}
The conditional mutual information extends this to the setting where a conditioning variables is present. The analogous expression for CMI is:

\[ I(X;Y|Z) = \int \int P_{XYZ} \log \frac{P_{XYZ}}{P_X P_{Y|Z}} \, dx \, dy \, dz \]  

(4)

In terms of the entropies, it can be expressed as follows:

\[ I(X;Y|Z) = H(X|Z) - H(X|Y,Z) \]  

(5)

\[ = H(Y|Z) - H(Y|X,Z) \]  

(6)

Both MI and CMI are special cases of a statistical quantity called KL-divergence, which measures how different one distribution is from another. The KL-divergence between two distributions \( P_X \) and \( Q_X \) is as follows:

\[ D_{KL}(P_X||Q_X) = \int P_X(x) \log \frac{P_X(x)}{Q_X(x)} \, dx \]  

(7)

In terms of the KL-divergence, we can express MI and CMI as follows:

\[ I(X;Y) = D_{KL}(P_{XY}||P_X P_Y) \]  

(8)

\[ I(X;Y|Z) = D_{KL}(P_{XY|Z}||P_X P_{Y|Z}) \]  

(9)

This definition of MI tries to capture how much the given joint distribution is different from \( X \) and \( Y \) being independent (respectively conditionally independent in case of CMI). The various estimators in the literature aim to utilize a particular expression of MI (or CMI), while avoiding computation of density functions explicitly. While KSG is based on the summation of entropy terms, MINE derives its estimates based on lower bounds of KL-divergence.

**Lower bounds of Mutual Information.** The following lower bounds of KL-divergence (hence also mutual information) were used in Belghazi et al. (2018) for the MINE estimator.

Donsker-Varadhan bound: This bound is tighter and is given by:

\[ D_{KL}(P||Q) = \sup_{R \in \mathcal{R}} \left( \mathbb{E}_P[R] - \log(\mathbb{E}_Q[e^R]) \right) \]  

(10)

f-divergence bound: A slightly loose bound is given by the following relation:

\[ D_{KL}(P||Q) = \sup_{R \in \mathcal{R}} \left( \mathbb{E}_P[R] - \mathbb{E}_Q[e^{R-1}] \right) \]  

(11)

The supremum in both the bounds (equation 10 and 11) is over all functions \( R \in \mathcal{R} \) such that the expectations are finite. MINE uses a neural network as a parameterized function \( R_{\phi} \), which is optimized with these bounds.

### 3.1 MIN-MAX FORMULATION FOR CMI

Building on top of these lower bounds, we further take resort to a variational form of conditional mutual information. Observing closely the expression for \( I(X;Y|Z) \) in equation 4, we find that samples need to be drawn from \( p(y|z) \) which is not available from given data \( (X,Y,Z) \) directly. One approach used in Mukherjee et al. (2019) is to learn \( p(y|z) \) using a conditional GAN, KNN or conditional VAE. Can we combine this step directly with the lower bound maximization?

We first note that the CMI expression can be upper bounded as follows:

\[ I(X;Y|Z) = D_{KL}(P_{XYZ}||P_X P_{Y|Z}) \]  

(12)

\[ = D_{KL}(P_{XY|z}||P_X Q_{Y|z}) \]  

\[ - D_{KL}(P_{Y|z}||Q_{Y|z}) \]  

\[ \leq D_{KL}(P_{XYZ}||P_X Q_{Y|z}) \]

since \( D_{KL}(P||Q) \geq 0 \). In equation 12 the equality is achieved when \( Q_{Y|z} = P_{Y|z} \) and we can express \( I(X;Y|Z) \) as

\[ I(X;Y|Z) = \inf_{Q_{Y|z}} D_{KL}(P_{XY|z}||P_X Q_{Y|z}) \]  

(13)

Equation 13 coupled with the Donsker-Varadhan bound (equation 10) leads to a min-max optimization for MI estimation as follows:

\[ I(X;Y|Z) = \inf_{Q_{Y|z}} \sup_{R \in \mathcal{R}} \left( \mathbb{E}_{s \sim P_{XYz}} [R(s)] - \log(\mathbb{E}_{s \sim P_{Xz}}[e^{R(s)}]) \right) \]  

(14)

Equation 14 offers a pragmatic approach for estimating CMI. Since neural nets are universal function approximators, it is a possibility to deploy one such network to approximate the variational distribution \( Q_{Y|z} \) and another for learning the regression function given by \( R \).

The following section provides a detailed narration of how to achieve this objective.

### 3.2 C-MI-GAN

To begin with, we elaborate different components of the proposed estimator - C-MI-GAN. As depicted in Figure 1 the variational distribution, \( Q_{Y|z} \) is parameterized using a network denoted as \( G_\theta \). In other words, \( G_\theta \) is capable of sampling from the distribution \( Q_{Y|z} \), hence it is called the generator network. The regression network, \( R_{\phi} \) parameterizes the function class on the R.H.S. of the Donsker-Varadhan identity (refer to equation 10). Gaussian noise concatenated with conditioning variable \( Z \) is fed as input to \( G_\theta \). \( R_{\phi} \) is trained with samples from
Figure 1: Block Diagram for C-MI-GAN (Best viewed in colour). Samples drawn from any simplistic noise distribution are concatenated with the samples from the marginal $P_Z$ and fed to the generator as input. The generated samples from the variational distribution $Q_{Y|Z}$ are then concatenated with samples from $P_{XZ}$ and given as input to the regression network along with samples from $P_{XYZ}$. $I(X; Y|Z)$ is obtained by negating the loss of the trained regression network.

$P_{XYZ}$ and $P_{XZ}Q_{Y|Z}$. During training, we optimize the regression network and the generator jointly using the objective function $h(Q_{Y|Z}, R)$ as defined below.

$$h(Q_{Y|Z}, R) = \inf_{Q_{Y|Z}} \sup_{R \in \mathcal{R}} \left( \int_{s_0}^{s_{\max}} P_{XYZ}R(s)ds - \log \left( \int_{s_0}^{s_{\max}} P_{XZ}Q_{Y|Z}e^{R(s)}ds \right) \right)$$

(15)

In each training loop, we optimize the parameters of $R_{\phi}$ and $G_{\theta}$, using a learning schedule and RMSProp optimizer. The detailed procedure is described in Algorithm [1]. Upon successful completion of training of the joint network, $G_{\theta}$ starts generating samples from the distribution $P_{Y|Z}$ and the output of the regression network converges to $I(X; Y|Z)$.

Next, we formally show that the alternate optimization of $R_{\phi}$ and $G_{\theta}$ optimizes the objective function defined in equation [15] and when the global optima is reached, the optimal value of the objective function coincides with CMI. To start with, we derive the expression for the optimal regression network and subsequently show that the optimal value of the objective function coincides with CMI under the optimal regression network.

**Theorem 1.** For a given generator, $G$, the regression network’s objective is to maximize the quantity $h(Q_{Y|Z}, R)$.

$$h(Q_{Y|Z}, R) = \int_{s_0}^{s_{\max}} P_{XYZ}R(s)ds - \log \left( \int_{s_0}^{s_{\max}} P_{XZ}Q_{Y|Z}e^{R(s)}ds \right)$$

(17)

For the optimum regression network, $R^*$,

$$\frac{\partial h}{\partial R} \bigg|_{R^*} = 0$$

$$\Rightarrow P_{XYZ} - \frac{P_{XZ}Q_{Y|Z}e^{R^*}}{\int P_{XZ}Q_{Y|Z}e^{R^*}ds} = 0$$

$$\Rightarrow \frac{P_{XZ}Q_{Y|Z}e^{R^*}}{P_{XYZ}} = \int P_{XZ}Q_{Y|Z}e^{R^*}ds = e^c$$

$$\Rightarrow R^* = \log \frac{P_{XYZ}}{P_{XZ}Q_{Y|Z}} + c$$

(18)

Now we show that with the optimal regression network $R^*$ we obtain the CMI by minimizing the objective function.

**Theorem 2.** $h(Q_{Y|Z}, R^*)$ achieves its minimum value $I(X; Y|Z)$, iff $Q_{Y|Z} = P_{Y|Z}$.

**Proof.** For a given generator, $G$, the regression network’s objective is to maximize the quantity $h(Q_{Y|Z}, R)$.

$$h(Q_{Y|Z}, R) = \int_{s_0}^{s_{\max}} P_{XYZ}R(s)ds - \log \left( \int_{s_0}^{s_{\max}} P_{XZ}Q_{Y|Z}e^{R(s)}ds \right)$$

For the optimum regression network, $R^*$, we obtain the CMI by minimizing the objective function defined in equation [15] and when the global optima is reached, the optimal value of the objective function coincides with CMI. To start with, we derive the expression for the optimal regression network and subsequently show that the optimal value of the objective function coincides with CMI under the optimal regression network.

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**Theorem 2.** $h(Q_{Y|Z}, R^*)$ achieves its minimum value $I(X; Y|Z)$, iff $Q_{Y|Z} = P_{Y|Z}$.
Since $D_{KL}(P_{Y|Z}||Q_{Y|Z}) \geq 0$, when $P_{Y|Z} = Q_{Y|Z}$, $D_{KL}(P_{Y|Z}||Q_{Y|Z}) = 0$ and the minimum value is $h(P_{Y|Z}, R^*) = I(X; Y|Z)$.

The alternate optimization of $R_\phi$ and $G_\theta$ is similar to the generative adversarial networks (Goodfellow et al. (2014)), in that they are both comprised of similar adversarial training procedure. However, C-MI-GAN significantly differs from traditional GAN in the following sense:

- The regression task is completely unsupervised as no target value is provided to the network during training.
- The proposed loss function to estimate CMI is foreign to traditional GAN literature.
- The binary discriminator in traditional GAN is replaced by a regression network, $R_\phi$ that estimates the CMI (refer to Figure 1).

Algorithm 1 Pseudo code for C-MI-GAN

Inputs: $D = \{x^{(i)}, y^{(i)}, z^{(i)}\}_{i=1}^m \sim P_{XYZ}$

Outputs: $I(X; Y|Z)$

1: function CMIGAN
2:     for $n \leftarrow 1$ to $N$ do
3:         Initialize $R_\phi$ and $G_\theta$
4:     for $i \leftarrow 1$ to training_steps do
5:         for $j \leftarrow 1$ to reg_training_ratio do
6:             Shuffle $D \sim P_{XYZ}$
7:             $D_b \leftarrow \{x^{(k)}\}_{k=1}^s \sim P_{XYZ}$
8:             noise $\leftarrow \{x^{(k)}\}_{k=1}^s \sim \mathcal{N}(0, I_{d_m})$
9:             $\{y^{(k)}_{y}\}_{k=1}^s \leftarrow G_\theta($noise, $Z_b$)
10:            $D_b \leftarrow \{x^{(k)}, y_{y}^{(k)}, z^{(k)}\}_{k=1}^s$
11:            $L_{reg} \leftarrow -E_{D_b}[R_\phi] + \log(E_{D_b}[e^{R_\phi}])$
12:            Minimize $L_{reg}$ and Update $\phi$
13:        end for
14:     for $n \leftarrow 1$ to gen_training_steps do
15:         Minimize $L_{gen}$ and Update $\theta$
16:         if $t \% lr\_schedule\_interval == 0$ then
17:             $\eta_{gen} \leftarrow \eta_{gen} \times decay\_rate$
18:             $\eta_{reg} \leftarrow \eta_{reg} \times decay\_rate$
19:         end if
20:     end for
21:     $\hat{I}_n(X; Y|Z) \leftarrow -L_{reg}$
22: end for
23: $\hat{I}(X; Y|Z) \leftarrow \frac{1}{N} \sum_{n=1}^N \hat{I}_n(X; Y|Z)$
24: end function

4 EXPERIMENTAL RESULTS

In this section we compare the CMI estimates, on different data sets, of our proposed method against the estimations of the state of the art CMI estimators such as f-MINE (Belghazi et al. (2018)) and CCMI (Mukherjee et al. (2019)). We design similar experiments on similar data sets as Mukherjee et al. (2019) to demonstrate the efficacy of our proposed estimator: C-MI-GAN. Unlike the method proposed in this work, the existing methods rely on a separate generator for generating samples from the conditional distribution. Therefore, “Generator”+“Divergence estimator” notation is used to denote the estimators used as baseline. For example, CVAE+f-MINE implies that Conditional VAE (Sohn et al. (2015)) is used for generating samples from $P_{Y|Z}$ and f-MINE (Belghazi et al. (2018)) is used for divergence estimation. MI difference based estimators are represented as MI-Diff.+“Divergence estimator”. For baseline models we have used the codes available in the repository of Mukherjee et al. (2019). Architecture for $R_\phi$ and $G_\theta$ and hyper-parameter settings for our proposed method are provided in the supplementary.

To illustrate the effectiveness of our proposed method we consider two types of data sets:

- Synthetically generated data sets having linear dependency.
- Synthetically generated data sets having non-linear dependency.

The most severe problem with the existing CMI estimators is that their performance drop significantly with increase in data dimension. To see how well the proposed estimator fares, compared to the existing estimators for high dimensional data, we vary the dimension, $d_z$ of the conditioning variable, $Z$ over a wide range, in both the data sets. However, in both the data sets $d_x = d_y = 1$, as found commonly in the literature on causal discovery and independence testing (Sen et al. (2017), Doran et al. (2014)). Nevertheless, the proposed method can easily be adapted to multi-dimensional $X$ and $Y$, as the networks $G_\theta$ and $R_\phi$ can accommodate varying input dimensions. Besides, we consider data sets having as low as 5k to as high as 50k samples to understand the behaviour of the estimators as sample complexity varies.

Ground Truth CMI: For the data sets with linear dependency, ground truth CMI can be computed by numerical integration. However, to the best of our knowledge, there is no analytical formulation to compute the ground truth CMI for the synthetic data sets with non-linear dependency. As a workaround to this issue, as
4.1 CMI ESTIMATION

4.1.1 Data Set With Linear Dependence

We consider the following data generative models.

• Model 1: $X \sim \mathcal{N}(0, 1); Z \sim \mathcal{U}(-0.5, 0.5)^{d_z}; \epsilon \sim \mathcal{N}(Z_1, 0.01); Y \sim X + \epsilon$.

In this model $X$ is sampled from standard normal distribution. Each dimension of $Z$ is drawn from a uniform distribution with support $[-0.5, 0.5]$. Finally $Y$ is obtained by perturbing $X$ with $\epsilon$, where $\epsilon$ comes from a Gaussian distribution having mean $Z_1$, the first dimension of $Z$ and variance 0.01. Therefore, the dependence between $X$ and $Y$ is through the first dimension of the conditioning variable $Z$.

• Model 2: $X \sim \mathcal{N}(0, 1); Z \sim \mathcal{N}(0, 1)^{d_z}; U = w^T Z; ||w||_1 = 1; \epsilon \sim \mathcal{N}(U, 0.01); Y \sim X + \epsilon$.

Unlike in model 1, here the dimensions of $Z$ comes from standard normal distribution and the mean of $\epsilon$ is weighted average of all the dimensions of $Z$. The weight vector $w$ is constant for a particular data set and varies across data sets generated by model 2.

To study the effect of sample size on the estimate we generate data by fixing $d_z = 20$ and $n \in$
Figure 3: This figure compares the performance of the different CMI estimators on all the 20 non linear data sets. However, due to very poor performance of “Generator”+“Classifier” estimators, we plot the estimates of “CVAE”+“Classifier” only as a representative of that class of estimators. Estimated CMI, averaged over 10 runs is plotted. Standard deviation is indicated with the thin dark lines on top of the bar plot. Like in the linear case, the proposed C-MI-GAN outperforms the state of the art estimators in terms of both average CMI estimation and variation in estimation (Best viewed in color).

\{5000, 10000, 20000, 50000\}. Next, we fix \(n = 20000\) and \(d_z \in \{1, 10, 20, 50, 100\}\) to observe the effect of dimension on the estimation.

Average estimate over 10 runs are reported for each estimator. As compared to the state of the art estimators, C-MI-GAN estimates are closer to the ground truth CMI. Also, the variations in estimate of C-MI-GAN over the 10 runs are significantly smaller as compared to the state of the art estimators.

4.1.2 Data Set With Non-Linear Dependence

Data generating model:

\[
Z \sim \mathcal{N}(1, I_{d_z}) \quad X = f_1(\eta_1) \quad Y = f_2(A_{zy}Z + A_{xy}X + \eta_2)
\]

Where, \(f_1, f_2 \in \{\cos(\cdot), \tanh(\cdot), \exp(-|\cdot|)\}\) and selected randomly; \(\eta_1, \eta_2 \sim \mathcal{N}(0, 0.1)\). The elements of the random vector \(A_{zy}\) are drawn independently from \(\mathcal{N}(0,1)\). The vector is then normalized to have unit norm. Since, \(d_x = d_y = 1\), \(A_{xy} = 2\) is a scalar.

To generate the data we consider all possible combinations of \(n \in \{5000, 10000, 20000, 50000\}\) and \(d_z \in \{10, 20, 50, 100, 200\}\), and obtain a set of 20 data-sets.

Figure 3 plots the average estimate of different estimators over 10 runs for all 20 data-sets. Error bar (standard deviation) is plotted as well on top of the estimation. As can be seen from the plot, only MI-Diff.+Classifier among the existing estimators provides reasonable estimate when \(d_z\) is high, while the proposed method track the true CMI more closely.

4.2 APPLICATION: CONDITIONAL INDEPENDENCE TESTING

To evaluate the proposed CMI estimator on an application, we consider testing the null hypothesis of conditional independence, used widely in conventional literature (Sen et al. (2017); Mukherjee et al. (2019)). The objective here is to decide, whether \(X\) and \(Y\) are independent given \(Z\) when we have access to samples from the joint distribution of the three variables. Formally, given samples from the distributions \(P(x,y,z)\) and \(Q(x,y,z)\) where \(Q(x,y,z) = P(x,z)P(y|z)\), we have to test our estimators on the hypothesis testing framework given by the null, \(H_0: X \perp Y | Z\) and the alternative, \(H_1: X \not\perp Y | Z\).

The conditional independence test setting will be used to test our estimator based on the fact that \(X \perp Y | Z \iff\)
\( I(X; Y | Z) = 0 \). A simple rule can thus be established: reject the null hypothesis if \( I(X; Y | Z) \) is greater than some threshold (to allow some tolerance in the estimation) and accept it otherwise.

This problem can be cast as binary classification problem where samples belong to either class-CI or class-CD. Therefore, area under ROC curve (AuROC) is a good metric to compare the performance of different algorithms. Therefore, in this endeavour of conditional independence testing, we consider the AuROC scores of different models for performance comparison.

### 4.2.1 Synthetic Data Set

For this experiment, data is generated using the post non-linear noise model as used by Sen et al. (2017) and Mukherjee et al. (2019). The data generation model for this experiment is:

\[
Z \sim \mathcal{N}(1, I_{d^z}) \\
X = \cos(a_x Z + \eta_1) \\
Y = \begin{cases} 
  \cos(b_y Z + \eta_2), & \text{if } X \perp Y | Z \\
  \cos(cX + b_y Z + \eta_2), & \text{otherwise}
\end{cases}
\]

\( \eta_1, \eta_2 \sim \mathcal{N}(0, 0.25); a_x, b_y \sim \mathcal{U}(0, 1)^{d_z} \) and normalized such that \( ||a_x||_2 = ||b_y||_2 = 1; c \sim \mathcal{U}(0, 2) \). As before the model parameters \( a_x, b_y \), and \( c \) are kept constant for a particular data set but varies across data sets. \( d_x = d_y = 1 \) and \( d_z \in \{1, 5, 20, 50, 70, 100\} \). 100 data sets consisting of 50 conditionally independent and 50 conditionally dependent data sets are generated for each \( d_z \). Sample size of each data set is fixed as \( n = 5000 \).

We compare the performance of our proposed method C-MI-GAN with CCIT (Sen et al. (2017)) and CCMI (Mukherjee et al. (2019)). As can be seen in Figure 4, performance of CCIT degrades rapidly as \( d_z \) increases. However, performance of C-MI-GAN and CCMI remains comparable for all \( d_z \). Performance of C-MI-GAN remains undeterred with increasing dimensions.

### 4.2.2 Flow-Cytometry: Real Data

To test the efficacy of our proposed method in conditional independence testing on real data, we used Flow cytometry dataset introduced by Sachs et al. (2005). This dataset quantifies the availability of 11 biochemical compounds in single human immune system cells under different test conditions.

The consensus network in Figure 5 depicting the causal relations between the 11 biochemical compounds has been considered as the ground truth.

The underlying concept for generating the CI and CD datasets is similar to that used in Sen et al. (2017) and Mukherjee et al. (2019). A node \( X \) is conditionally independent of any other unconnected node \( Y \) given its Markov blanket i.e. its parents, children and co-parents of children. So given \( Z \) consisting of the parents, children and co-parents of children of \( X \), \( X \) is conditionally independent of any other node \( Y \). Also, if a direct edge exists between \( X \) and \( Y \), then given any \( Z \), \( X \) is not conditionally independent of \( Y \). We have used this philosophy to create 70 CI and 54 CD data sets.

Figure 5: Consensus network, according to Sachs et al. (2005).

![Consensus network](image)

Figure 4: Performance of CCIT degrades with \( d_z \). CCMI and C-MI-GAN are comparable across all \( d_z \). (Best viewed in color).

We compare the performance of our proposed method C-MI-GAN with CCIT (Sen et al. (2017)) and CCMI (Mukherjee et al. (2019)). As can be seen in Figure 4, performance of CCIT degrades rapidly as \( d_z \) increases. However, performance of C-MI-GAN and CCMI remains comparable for all \( d_z \). Performance of C-MI-GAN remains undeterred with increasing dimensions.

The consensus network in Figure 5 depicting the causal relations between the 11 biochemical compounds has been considered as the ground truth.

The underlying concept for generating the CI and CD datasets is similar to that used in Sen et al. (2017) and Mukherjee et al. (2019). A node \( X \) is conditionally independent of any other unconnected node \( Y \) given its Markov blanket i.e. its parents, children and co-parents of children. So given \( Z \) consisting of the parents, children and co-parents of children of \( X \), \( X \) is conditionally independent of any other node \( Y \). Also, if a direct edge exists between \( X \) and \( Y \), then given any \( Z \), \( X \) is not conditionally independent of \( Y \). We have used this philosophy to create 70 CI and 54 CD data sets.

Sachs et al. (2005) and Mooij and Heskes (2013) used a subset of 8 of the available 14 original flow cytometry data sets in their experiments to come up with Bayesian networks representing the underlying causal structure. We also used those 8 data sets in our experiments which had a combined total of around 7000 samples. The dimension of \( Z \) varies in the range 3 to 8.
CCIT obtains a mean AuROC score of 0.728, CCMI obtains a mean of 0.62 while C-MI-GAN outperforms both of them with a mean AuROC score of 0.798 (Best viewed in color).

As before, we compare again the AuROC score of C-MI-GAN against the scores of CCMI and CCIT and the results are plotted in Figure 6. C-MI-GAN retains its superior performance when compared against CCMI and CCIT. Surprisingly, CCIT outperforms CCMI, which contradicts the result presented by Mukherjee et al. (2019). This discrepancy might be due to limited capacity of their model architecture. We have created a larger data set consisting of around 7000 samples. Whereas, the numbers reported by Mukherjee et al. (2019) are based on a smaller subset consisting of 853 data points. A larger network might improve the performance of CCMI.

5 DISCUSSION OF RESULTS AND CONCLUSION

In this work, we propose a novel CMI estimator, C-MI-GAN. This estimator is based on the formulation of CMI as a min-max objective that can be optimized using joint training. We refrain from estimating two separate MI terms that could have unequal bias present. As opposed to separately training a conditional sampler and a divergence estimator, which may be sub-optimal, our joint training incorporates both steps into a single training procedure. We find that the estimator obtains improved estimates over a range of linear and non-linear data sets, across a wide range of dimension of the conditioning variable and sample size. Finally, we achieve performance boost in CI testing on simulated and real data sets using our improved estimator.

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Table 1: Hyperparameters: CMI Estimation

| Hyperparameters          | Regressor | Generator |
|-------------------------|-----------|-----------|
| # Hidden layers          | 2         | 2         |
| Hidden Units             | [128, 32] | [256, 64] |
| Activation: Hidden Layers| ReLu      | ReLu      |
| Activation: Final Layer  | Identity  | Identity  |
| Batch Size               | 4096      | 4096      |
| Initial Learning rate    | $5 \times 10^{-5}$ | $5 \times 10^{-5}$ |
| Optimizer                | RMSprop   | RMSprop   |
| # Training Steps         | 30k       | 30k       |
| $d_k$ to Noise dim. ratio| -         | 4         |
| Noise distribution       | $N(0, I_{d_k})$ | $N(0, I_{d_k})$ |
| Learning rate scheduling interval | 2k    | 2k        |
| Learning rate decay factor| 10       | 10        |

Table 2: Hyperparameters: CIT Application

| Hyperparameters          | Regressor | Generator |
|-------------------------|-----------|-----------|
| # Hidden layers          | 3         | 3         |
| Hidden Units             | [128, 32, 8] | [128, 64, 16] |
| Activation: Hidden layers | ReLu      | ReLu      |
| Activation: Final layer  | Identity  | Identity  |
| Batch Size               | 4096      | 4096      |
| Initial Learning rate    | 0.001     | 0.001     |
| Optimizer                | RMSprop   | RMSprop   |
| # Training Steps         | 10k       | 10k       |
| Learning rate decay checkpoint | 2k    | 2k        |
| Learning rate decay factor| 10       | 10        |

7 MI-GAN

Ideas presented in [31] in the main paper can be applied to estimating mutual information as well.

$$I(X; Y) = D_{KL}(P_{XY} || P_X P_Y)$$

$$= D_{KL}(P_{XY} || P_X Q_Y) - D_{KL}(P_Y || Q_Y)$$

$$\leq D_{KL}(P_{XY} || P_X Q_Y)$$ (20)

In equation (20), the equality is achieved when $Q_Y = P_Y$ and it may be expressed as

$$I(X; Y) = \inf_{Q_Y} D_{KL}(P_{XY} || P_X Q_Y)$$ (21)

Equation (21) coupled with the Donsker-Varadhan bound leads to a min-max optimization for MI estimation as below.

$$I(X; Y) = \inf_{Q_Y} \sup_{R \in \mathcal{R}} \left( \mathbb{E}_{s \sim P_{XY}} [R(s)] - \log \left( \mathbb{E}_{s \sim P_{XQ_Y}} [e^{R(s)}] \right) \right)$$ (22)

Here we consider a simple setting of two correlated gaussian random variables in $2n$ dimensions, $(X, Y) \sim \mathcal{N}(\overrightarrow{0}_{2n \times 1}, \Sigma = (I_{n \times n} \rho I_{n \times n})$) and estimate $I(X; Y)$ using the min-max formulation as mentioned in equation (22). Next, we compare the results with the existing estimators. Figures 7a and 7b plots the estimated mi using MI-GAN, Classifier MI and f-MINE.
7.1 DIFFERENCE BASED MIN-MAX FORMULATION FOR CMI

Conditional mutual information can be expressed as difference of two mutual information as below:

$$I(X;Y|Z) = I(X;YZ) - I(X;Z)$$ (23)

Equation 22 and equation 23 together leads to another min-max formulation of $I(X;Y|Z)$ requiring one generator and two regression networks.

$$I(X;Y|Z) = \inf_{Q_X} \left( \sup_{R_1 \in \mathcal{R}} \left( \mathbb{E}_{s \sim P_{XYZ}} [R_1(s)] - \log \mathbb{E}_{s \sim Q_X P_{YZ}} [e^{R_1(s)}] \right) - \sup_{R_2 \in \mathcal{R}} \left( \mathbb{E}_{s \sim P_{XZ}} [R_2(s)] - \log \mathbb{E}_{s \sim Q_X P_{Z}} [e^{R_2(s)}] \right) \right)$$ (24)

We call the estimator based on difference based min-max formulation for CMI (equation 24) as MI-Diff.-GAN. We evaluate the model on the synthetic data sets proposed in Sections 4.1.1 and 4.1.2. In Figures 8 and 9, we compare the results of MI-Diff.-GAN with the existing difference based CMI estimators. However a detailed comparison of MI-Diff.-GAN with all other state of the art estimators has been tabulated in Tables 3, 4 and 5, which comprise of the average estimated CMI and the variance in the estimation, calculated over 10 runs, corresponding to each of the estimators discussed in this work. Moreover, the RMSE calculated between the true cmi and the average estimated cmi values for each of the estimators, have been highlighted in Table 6. It can serve as a naive performance metric for the estimators.

From the results obtained from the various experimental setups discussed in this work, it is apparent that MI-Diff.-GAN and C-MI-GAN are at par with each other and superior to the existing CMI estimators in terms of accuracy in CMI estimation and variation in estimates.
Figure 9: Performance of MI-Diff-GAN on the data generated using non linear models proposed in 4.1.2. Again we compare against MI-Diff based CMI estimators such as MI-Diff. + Classifier and MI-Diff. + f-MINE. Average over 10 runs is plotted. Variation in the estimates are measured using standard deviation and are highlighted in the plots using the thin dark lines on top of the bar plots. MI-Diff-GAN performs better in terms of both estimation accuracy and variation in estimates. (Best viewed in color)

Table 3: Results Of CMI Estimation On Linear Model I

| $d_s$ | $n$ | Avg. | Std. | Avg. | Std. | Avg. | Std. | Avg. | Std. | Avg. | Std. | Avg. | Std. | True CMI |
|-------|-----|------|------|------|------|------|------|------|------|------|------|------|--------|
| 20    | 5   | 1.936| 0.126| 1.992| 0.171| 1.985| 0.105| 1.283| 0.027| 2.348| 0.004| 2.314| 0.004| 2.329903976 |
| 20    | 10  | 1.963| 0.157| 1.947| 0.113| 2.064| 0.049| 1.85 | 0.078| 2.314| 0.004| 2.173| 0.004| 2.329903976 |
| 20    | 20  | 2.091| 0.074| 2.041| 0.066| 2.131| 0.036| 2.074| 0.075| 2.306| 0.003| 2.24  | 0.004| 2.329903976 |
| 20    | 50  | 2.195| 0.051| 2.204| 0.051| 2.158| 0.028| 2.217| 0.02  | 2.06 | 0.338| 2.318 | 0.003| 2.298 | 0.003| 2.329903976 |
| 50    | 1   | 2.304| 0.08 | 2.261| 0.058| 2.264| 0.084| 2.244| 0.046| 2.248| 0.042| 2.318 | 0.002| 2.314 | 0.003| 2.324202061 |
| 10    | 20  | 2.229| 0.066| 2.207| 0.087| 2.162| 0.084| 2.235| 0.046| 2.208| 0.065| 2.323 | 0.003| 2.294 | 0.002| 2.32732899 |
| 20    | 10  | 1.744| 0.09 | 1.631| 0.081| 1.651| 0.07 | 1.962| 0.037| 1.524| 0.237| 2.323 | 0.007| 2.159 | 0.004| 2.318082313 |
| 20    | 100 | 1.423| 0.117| 1.103| 0.109| 1.141| 0.084| 1.678| 0.058| 0   | 0   | 2.379 | 0.011| 2.035 | 0.012| 2.333104637 |

Table 4: Results Of CMI Estimation On Linear Model II

| $d_s$ | $n$ | Avg. | Std. | Avg. | Std. | Avg. | Std. | Avg. | Std. | Avg. | Std. | Avg. | Std. | True CMI |
|-------|-----|------|------|------|------|------|------|------|------|------|------|------|------|--------|
| 20    | 5   | 2.039| 0.13 | 1.895| 0.103| 1.998| 0.093| 2.058| 0.082| 0.886| 0.047| 2.402| 0.018| 2.127 | 0.011| 2.324819809 |
| 20    | 10  | 2.037| 0.091| 1.99 | 0.074| 2.02 | 0.111| 2.106| 0.076| 1.627| 0.051| 2.34  | 0.015| 2.207 | 0.006| 2.324819809 |
| 20    | 20  | 2.098| 0.058| 2.067| 0.083| 2.14 | 0.089| 2.123| 0.054| 2.071| 0.054| 2.36  | 0.006| 2.257 | 0.004| 2.324819809 |
| 20    | 50  | 2.218| 0.045| 2.162| 0.035| 2.239| 0.013| 2.183| 0.031| 2.124| 0.04  | 2.291 | 0.005| 2.274 | 0.003| 2.324819809 |
| 50    | 1   | 2.29 | 0.07 | 2.251| 0.042| 2.231| 0.068| 2.254| 0.033| 2.204| 0.046| 2.312 | 0.002| 2.309 | 0.001| 2.313665532 |
| 10    | 20  | 2.189| 0.052| 2.167| 0.033| 2.225| 0.044| 2.192| 0.041| 2.144| 0.053| 2.3   | 0.004| 2.28  | 0.003| 2.325076241 |
| 50    | 20  | 1.713| 0.096| 1.63 | 0.071| 1.762| 0.081| 1.952| 0.019| 1.605| 0.159| 2.355 | 0.005| 2.191 | 0.006| 2.318283481 |
| 100   | 20  | 1.358| 0.122| 1.2  | 0.095| 1.368| 0.107| 1.66 | 0.042| 0.314| 0.176| 2.44  | 0.01  | 2.086 | 0.006| 2.324413766 |
Table 5: Results Of CMI Estimation On Non linear Model

| $d$ | $n$ | CGAN+Classifier | CVAE+Classifier | KNN+Classifier | MI-Diff.+Classifier | MI-Diff.+f-MINE | C-MI-GAN | MI-Diff-GAN | True CMI |
|-----|-----|-----------------|-----------------|----------------|---------------------|----------------|----------|------------|----------|
| 10  | 5   | 0.655           | 0.622           | 0.303          | 0.295               | 0.304          | 0.19     | 0.291      | 0.412    |
| 10  | 10  | 0.26            | 0.243           | 0.02           | 0.026               | 0.032          | 0.022    | 0.253      | 0.287     |
| 10  | 20  | 0.116           | 0.076           | 0.012          | 0.084               | 0.056          | 0.017    | 0.056      | 0.061     |
| 10  | 50  | 0.124           | 0.076           | 0.007          | 0.088               | 0.006          | 0.007    | 0.007      | 0.006     |
| 20  | 5   | 0.387           | 0.184           | 0.03           | 0.212               | 0.054          | 0.229    | 0.035      | 0.051     |
| 20  | 10  | 0.261           | 0.058           | 0.287          | 0.024               | 0.026          | 0.024    | 0.224      | 0.284     |
| 20  | 20  | 0.322           | 0.06            | 0.337          | 0.024               | 0.029          | 0.29     | 0.015      | 0.331     |
| 20  | 50  | 0.511           | 0.157           | 0.518          | 0.061               | 0.385          | 0.012    | 0.368      | 0.011     |
| 50  | 5   | 0               | 0.054           | 0.064          | 0.033               | 0.021          | 0.148    | 0.04       | 0.014     |
| 50  | 10  | 0.471           | 0.131           | 0.343          | 0.085               | 0.358          | 0.524    | 0.026      | 0.518     |
| 50  | 20  | 0.005           | 0.011           | 0              | 0                   | 0              | 0.008    | 0.008      | 0.016     |
| 50  | 50  | 0.42            | 0.083           | 0.402          | 0.049               | 0.28           | 0.013    | 0.272      | 0.007     |
| 100 | 5   | 0               | 0               | 0              | 0                   | 0              | 0.007    | 0.013      | 0.007     |
| 100 | 10  | 2.122           | 3.531           | 0              | 0                   | 0              | 0.042    | 0.041      | 0.045     |
| 100 | 20  | 0               | 0.011           | 0.025          | 0.038               | 0.022          | 0.023    | 0.028      | 0.033     |
| 100 | 50  | 0               | 0               | 0              | 0                   | 0              | 0.001    | 0.001      | 0.004     |
| 200 | 5   | 0               | 0               | 0              | 0                   | 0              | 0.023    | 0.061      | 0.016     |
| 200 | 10  | 0               | 0               | 0              | 0                   | 0              | 0.058    | 0.072      | 0         |
| 200 | 20  | 0               | 0               | 0              | 0                   | 0              | 0.054    | 0.036      | 0.076     |
| 200 | 50  | 0               | 0               | 0              | 0                   | 0              | 0.169    | 0.024      | 0         |

Table 6: CMI Estimation: RMSE Computed Over Different Models

| Models          | CGAN+Classifier | CVAE+Classifier | KNN+Classifier | MI-Diff.+Classifier | MI-Diff.+f-MINE | C-MI-GAN | MI-Diff-GAN |
|-----------------|-----------------|-----------------|----------------|--------------------|----------------|----------|-------------|
| Linear Model I  | 0.439951        | 0.556009        | 0.539935       | 0.319044           | 0.971969       | 0.020806 | 0.166482    |
| Linear Model II | 0.439715        | 0.519229        | 0.430447       | 0.311608           | 0.952448       | 0.053325 | 0.130044    |
| Non Linear Model| 0.49818         | 0.290552        | 0.299482       | 0.228215           | 0.241488       | 0.119516 | 0.099798    |