A saturating lower confidence bound for mutual information based on classification error

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Abstract

Estimating the mutual information $I(X;Y)$ based on observations becomes statistically infeasible in high dimensions without some kind of modeling assumption. One approach is to assume a parametric joint distribution on (X,Y), but in many applications, such a strong modeling assumption cannot be justified. An alternative approach is to obtain a lower bound on the mutual information based on a classification task. Existing methods include lower confidence bounds based on the confusion matrix of the classifier, as well as Fano's inequality and its generalizations. One might hope that if the classifier is *consistent*, in the sense that the classification error approaches the Bayes error in the large-sample limit, that the information lower bound $\underline{I}(X,Y)$ should also approach the true information $I(X;Y)$. However, existing methods always produce a bound which is on the order $O(\log k)$, where K is the number of classes, so when $I(X;Y) \gg \log k$, the lower confidence bound is inconsistent even when the classifier is consistent. On the other hand, consistency is not possible with a fixed number of classes since the full distribution of X is not revealed. In this paper, we construct a novel lower bound based on high-dimensional asymptotics; our proposed bound satisfies a weaker property than consistency, called *saturation.* A saturating lower bound has the property that as $I(X;Y)$ and the number of observations grow to infinity (while the number of classes K stays fixed,) that $\underline{I}((X,Y)) = O(I(X,Y))$, assuming that the classifier used is consistent. While the theory is based on a large-sample, high-dimensional limit, we demonstrate through simulations that our proposed lower confidence bound has superior performance to the alternatives in problems of moderate dimensionality.

1 Introduction

Mutual information $I(X;Y)$ is fundamentally a measure of dependence between random variables X and Y, and is defined as

$$I(X;Y) = \int p(x,y) \log \frac{p(x,y)}{p(x)p(y)} dxdy.$$

In its original context of information theory, the mutual information describes the rate at which a noisy communications channel Y can communicate bits from a source stream X, but by now, the quantity $I(X,Y)$ has found many new uses in science and engineering. Mutual information is used to test for conditional independence, to quantifying the information between a random stimulus X and the signaling behavior of an ensembles of neurons, Y (Borst 1999); for use as an objective function for

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training neural networks (CITE), for feature selection in machine learning, and even as an all-purpose nonlinear measure of "correlation for the 21st century" (Speed.) What is common to all of these new applications, and what differs from the original setting of Shannon's theory of information, is that the variables X and Y have unknown distributions which must be inferred from data. In the case when X and Y are both low-dimensional, for instance, when summarizing the properties of a single neuron in response to a single stimulus feature, $I(X;Y)$ can be estimated nonparametrically using a reasonable number of observations. There exists a huge literature on nonparametric estimation of entropy and mutual information exists, see (CITE) for a review.

However, for high-dimensional X and Y the sample complexity grows exponentially with the dimension, making nonparametric approaches intractable in applications with high-dimensional data. One such application includes multivariate pattern analysis (MVPA), an area of neuroscience research pioneered by Haxby (2001), which studies how entire regions of the human brain respond to stimuli, using function magnetic resonance imaging (fMRI) data; in MVPA studies, the input X could be a natural image parameterized by $p = 10000$ image features, while the output Y is a $q = 20000$-dimensional vector of brain activation features obtained from the fMRI scan. In problems of such dimensionality, one can tractably estimate mutual information by assuming a multivariate Gaussian model: however, this approach essentially assumes a linear relationship between the input and output, and hence fails to quantify nonlinear dependencies. Rather than assuming a full parametric generative model, one can empirically select a good *discriminative* model by using machine learning. Treves (1997) first proposed using the empirical mutual information of the classification matrix in order to obtain a lower bound of the mutual information $I(X;Y)$; this confusion-matrix-based lower bound has subsequently enjoyed widespread use in the MVPA literature (Quiroga 2009.) But even earlier that this, the idea of linking classification performance to mutual information can be found in the beginnings of information theory: after all, Shannon's original motivation was to characterize the minimum achievable error probability of a noisy communication channel. More explicitly, Fano's inequality provides a lower bound on mutual information in relation to the optimal prediction error, or Bayes error. Fano's inequality can be further refined to obtain a tighter lower bound on mutual information (Tebbe and Dwyer 1968.) How do these different classification-based methods for lower bounding mutual information compare, to each other, and to nonparametric and parametric estimators of mutual information? Before discussing such comparisons, we must first delineate a number of assumptions on the sampling regime, and the properties of the classifiers.

1.1 Sampling assumptions

Assume that the variables X, Y have a joint distribution F, and that one can define a conditional distribution of Y given X,

$$Y|X \sim F_X,$$

and let G denote the marginal distribution of X. We consider two different types of sampling procedures:

- *pair sampling*: For $i = 1, \ldots, n$, the data (X^i, Y^i) are sampled i.i.d. from the joint distribution of (X, Y).
- *stratified sampling*: For $j = 1, \ldots, k$, sample i.i.d. *exemplars* $X^{(1)}, \ldots, X^{(k)} \sim G$. For $i = 1, \ldots, n$, draw Z^i iid from the uniform distribution on $1, \ldots, k$, then draw Y^i from the conditional distribution $F_{X^{(Z_i)}}$.

Pair sampling occurs in observational studies, where one observes both X and Y externally. On the other hand, stratified sampling is more commonly seen in controlled experiments, where an experimenter chooses an input X to feed into a black box, which outputs Y. An example from fMRI studies is an experimental design where the subject is presented a stimulus X, and the experimenter measures the subject's response via the brain activation Y.

Mutual information can be defined for discrete or continuous random variables (X, Y), or a combination of discrete input X and continuous output Y and vice-versa. Shannon's original paper (CITE) begins with the case of discrete X and discrete Y, and he considers the problem of decoding X from Y; this is the same problem as labelling a feature vector Y with class labels taking the possible values of X. In the case that X is uniformly distributed on its support, Fano's inequality provides a link between mutual information and classification via

$$I(X;Y) \leq (1 - e_{class}) \log K + ...$$

where e_{class} is the Bayes error and K is the size of the support of X. Since the generalization error of any classifier is greater than the Bayes error, Fano's inequality also holds when e_{class} is taken to mean the generalization error of the classifier. However, the generalization error of any classifier is an unknown parameter: at best, we can obtain upper and lower confidence bounds. If $\bar{e}$ is an α-upper confidence bound, in the sense that

$$\Pr[\bar{e} < e_{gen}] \leq \alpha,$$

then substituting $\bar{e}$ into Fano's inequality yields the lower confidence bound for mutual information,

$$\underline{I}_{Fano} = \log k + ...$$

In the discrete case, there is little consequence to the distinction between pair sampling and stratified sampling as long as the number of sampled classes k is much larger than the support of X. However, in the case of continuous X, the classification tasks must be defined differently depending on the sampling scheme. Under pair sampling, one can no longer take distinct inputs X to define distinct classes, since the notion of generalization error depends on repeated sampling from the same class. Instead, one can define a fixed number classes by specifying a partition on the support of X. For instance, in fMRI imaging experiments, the experimenter may divide a set of stimuli into intuitive categories (car, dog, person, etc.) In contrast, under stratified sampling, one can take the distinct exemplars $X^{(1)}, \ldots, X^{(k)}$ to define distinct classes. While there is no need to specify an arbitrary partition on the input space, the k classes will now be *randomly* defined. One consequence is that the Bayes error e_{Bayes} is a random variable: when the sampling produces k similar exemplars, e_{Bayes} will be higher, and when the sampling produces well-separated exemplars e_{Bayes} may be lower. For this reason, Fano's inequality no longer produces a lower bound–it could produce an overestimate of $I(X;Y)$ for an exceptionally well-separated exemplar set.

Most nonparametric estimators of $I(X;Y)$ are derived under the pair sampling assumption, and may perform badly in the stratified sampling case. On the other hand, there exist nonparametric estimators which are specialized for stratified sampling. Using the fact that

$$I(X;Y) = H(Y) - H(Y|X),$$

one can estimate $I(X;Y)$ by first estimating $H(Y)$ from the empirical marginal distribution of Y, and then estimating $H(Y|X)$ from the distributions within each class:

$$\hat{H}(Y|X) = \frac{1}{k}\sum_{i=1}^{k} \hat{H}(Y|X^{(i)})$$

After Gastpar et al. (2009), we call the resulting estimator $\hat{I}_0$. In their paper, Gastpar et al. showed that $\hat{I}_0$ is biased downwards due to undersampling of the exemplars; to counteract this bias, they introduce the anthropic correction estimator $\hat{I}_\alpha$. If the parameter $\alpha \in [0, 1)$ is chosen correctly, the estimator is unbiased, but no method is given to tune the parameter.

Parametric estimators tend to work similarly in either type of sampling, as long as the sampling is correctly accounted for in the likelihood model. For instance, Gastpar et al. combined their anthropic correction estimator with a gaussian model to estimate information in a high-dimensional dataset.

The most straightforward type of comparison that can be made is between different estimators (or confidence bounds) which use the same type of sampling. But when designing an experiment, a researcher may have a choice between a pair sampling design and a stratified sampling design. The cost of the design may depend simply on the total number of observations n, or there might be an extra cost associated with the number of unique exemplars k; or the opposite could be true–it may cost extra to obtain repeats from the same class. We make an initial stab at the topic of experimental design in our simulation study, with the assumption that the total number of observations n is constrained.

Our primary tool for comparing different estimators (or lower bounds) of mutual information will be through simulation studies, though we will outline some general ideas about the strengths and weaknesses of the three big modeling approaches–nonparametric, parametric, and discriminative–in the discussion.

The main subject of the paper, however, is our proposal of a new lower confidence bound based on classification error. In the following subsection we outline the assumptions and criteria we use in comparing methods *within* the family of classification-based estimators.

1.2 Classification

Formally, a classification rule is any (possibly stochastic) mapping $f : \mathcal{Y} \to \{1, \ldots, k\}$. The *generalization error* of the classification rule for classes $x^{(1)}, \ldots, x^{(k)}$ is

$$e_{gen}(f) = \frac{1}{k} \sum_{i=1}^{k} \Pr[f(Y) \neq i | X = x^{(i)}].$$

A trivial classification rule which outputs the result of a k-sided die roll for all inputs y would achieve a generalization error of $e_{gen} = \frac{k-1}{k}$. Conversely, even a single counterexample with $e_{gen} < \frac{k-1}{k}$ is indicative that y contains nonzero information about x. Hence, in order to demonstrate that y is informative of x, one tests the null hypothesis

$$H_0 : e_{gen}(f) = \frac{k-1}{k}$$

versus the alternative

$$H_1 : e_{gen}(f) < \frac{k-1}{k}.$$

Rejecting the null hypothesis for a given classification rule f can be taken as evidence that y is informative of x.

We have not yet specified how any classification rule f is to be obtained. Unless one has strong prior knowledge about the nature of the brain encoding, it is necessary to choose the function f in a data-dependent way in order to obtain a reasonable classification rule. A wide variety of machine learning algorithms exist for "learning" good classification rules f from data. We use the terminology *classifier* to refer to any algorithm which takes data as input, and produces a classification rule f as output. The following discussion makes it necessary for us to make a precise distinction between the *classifier* and the *classification rule* it produces, and our usage of the terms may differ from the standard in the literature. Mathematically speaking, the classifier is a functional which maps a set of observations to a classification rule,

$$\mathcal{F} : \{(x^1, y^1), \ldots, (x^m, y^m)\} \mapsto f(\cdot).$$

The data $(x^1, y^1), \ldots, (x^m, y^m)$ used to obtain the classification rule is called *training data.* When the objective is to obtain the best possible classification rule, as is the case in diagnostic settings, it is optimal to use all of the availible data to train the classifier. However, when the goal is to obtain *inference* about the performance of the classification rule, it beomes necessary to split the data into two independent sets: one set to train the classifier, and one to evaluate the performance. The reason that such a splitting is necessary is because using the same data to test and train a classifier introduces significant bias into the empirical classification error.

While tests of the generalization error suffice to establish the presence of information, the generalization error is less satisfactory as a measure of the information between X and Y, because e_{gen} depends on the classification rule f obtained–but since the performance of the classifier may vary depending on the choice of model (k-nearest neighbors, SVM, etc.) and the choice of tuning parameters, the quantity e_{gen} is therefore not uniquely defined. To resolve the ill-definedness of the generalization error, we define the Bayes error, which is simply the *optimal* generalization error

$$e_{Bayes} = \min_{f} e_{gen}(f).$$

Due to Bayes' theorem, the optimal classification rule f^* which achieves the Bayes error can be given explicitly: it is the maximum a posteriori (MAP) rule

$$f^*(y) = \text{argmax}_{i=1}^{k}\, p(y|x^{(i)}).$$

Of course, it is not possible to construct this rule in practice since the joint distribution is unknown. Instead, a reasonable approach is to try a variety of classifiers, producing rules $f_1, \ldots, f_m$, and taking the best generalization error as an estimate of the Bayes error. We give more details of this approach in the Discussion.

Under the assumption of randomized design, we treat the stimuli $x_1, \ldots, x_k$ as independent draws from some distribution $p(x)$. Defining the joint distribution of the stimulus X and the response Y as

$$p(x, y) = p(x)p(y|x),$$

one can also define the mutual information

$$I(X;Y) = \int p(x,y) \log \frac{p(x,y)}{p(x)p(y)} dxy.$$

In contrast the case of fixed design, the randomized design framework provides a principled way of making inferences about the population of stimuli exemplars, beyond the particular exemplars that were chosen for the study. This is particularly relevant for complex stimuli, for which the number of distinct stimuli species (e.g. distinct faces) could be astonomically large (i.e. the number of faces that a human could distinguish.) The concept of information $I(X;Y)$ captures the notion of the "complexity" of the stimuli representation. By inferring the information $I(X;Y)$, we make inferences about the complexity of the representation in the given brain region Y.

Methodologies for estimating mutual information under the assumption of randomization have been studied in (Borst 1999), (Nelken 2005) and most notably (Gastpar 2010); the latter studies the problem under an identical setup to ours. In addition to these approaches, one can obtain a lower bound on the information using the mutual information of the confusion matrix (Treves et al), (Quiroga 2009). In Section 3, we present our methodology for inferring mutual information under the randomized stimuli design setting.

Before presenting our approach, we first define the notion of average Bayes error, which is fundamental to our approach. The motivation for defining average Bayes error is the fact that the quantity e_{Bayes} is not a parameter of the joint distribution $p(x,y)$, but rather depends on the specific exemplars $x_1, \ldots, x_k$ selected; hence, one may write $e_{Bayes}(x_1, \ldots, x_k)$ to emphasize this dependence. The *average* Bayes error, on the other hand, is defined uniquely for any joint distribution,

$$e_{ABE,k} = \mathbf{E}[e_{Bayes}(X_1, \ldots, X_k)], \tag{1}$$

where $X_1, \ldots, X_K$ are drawn i.i.d. from $p(x)$. Supposing that an unbiased estimator for Bayes error $\hat{e}_{Bayes}$ exists, then $\hat{e}_{Bayes}$ will also be unbiased for $e_{ABE,k}$ under the randomization assumption. We show that under certain conditions, the average Bayes error can be well-approximated as a monotonically decreasing function of the mutual information, and vice-versa.

[[remove stuff abot testing, add def of saturation]]

2 Theory

Our goal in this section is to establish a relationship between the mutual information $I(X;Y)$ and the k-class average Bayes error, $e_{ABE,k}$. In short, we will identify a function π_k (which depends on k),

$$e_{ABE,k} \approx \pi_k(\sqrt{2I(X;Y)})$$

and that this approximation becomes accurate under a limit where $I(X;Y)$ is small relative to the dimensionality of X, and under the condition that the components of X are approximately independent. Formal conditions are given in the proof statement.

The function π_k is given by

$$\pi_k(c) = 1 - \int_{\mathbb{R}} \phi(z-c)\Phi(z)^{k-1} dz.$$

Figure 1 displays the plot of π_k for several values of k. For all values of k, $\pi_k(\mu)$ is monotonically decreasing in μ, and tends to zero as $\mu \to \infty$. This should not be surprising, because if $I(X;Y)$ is large, then the average Bayes error should be small. Another fact, which can be verified through a simple calculation, is that

$$\pi_k(0) = 1 - \frac{1}{k}.$$

This should also not be surprising, since if $I(X;Y) = 0$, then it should not be possible to obtain a classification rule which is better than guessing at random, which is only correct with probability $1/k$.

First, let us rewrite $e_{ABE,k}$ in terms of the joint density $p(x,y)$. Recall that the Bayes rule is

$$e_{Bayes}(x_1, \ldots, x_k) = \frac{1}{k} \sum_{i=1}^{k} \Pr[\hat{X}(Y) \neq x_i | X = x_i].$$

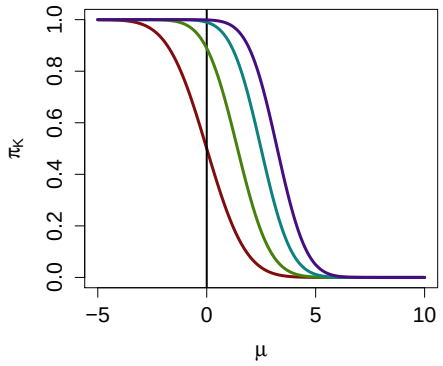


Figure 1: The function $pi_k(\mu)$, for $k = \{2, 9, 99, 999\}$ (left to right)

In turn, the Bayes classification rule is given in terms of the conditional density:

$$\hat{X}(y) = \text{argmax}_{x \in \{x_1,\ldots,x_k\}} p(y|x).$$

Therefore, we obtain

$$e_{Bayes}(x_1, \ldots, x_k) = \frac{1}{k} \sum_{i=1}^{k} \Pr[p(Y|x_i) \leq \max_{j \neq i} p(Y|x_j) | X = x_i].$$

In turn the average Bayes error can be written as

$$\begin{aligned} e_{ABE,k} &= \mathbf{E}[e_{Bayes}(X_1, \ldots, X_k)] && (2)\\ &= \frac{1}{k} \sum_{i=1}^{k} \mathbf{E}[\Pr[p(Y|x_i) \leq \max_{j \neq i} p(Y|x_j) | X = x_i]] && (3)\\ &= \mathbf{E}[\Pr[p(Y|x_1) \leq \max_{j \neq 1} p(Y|x_j) | X = x_1]] && (4)\\ &= \Pr[p(Y|X_1) \leq \max_{j \neq 1} p(Y|X_j) | X = X_1]. && (5) \end{aligned}$$

Defining $Z_i = \log p(Y|X_i) - \log p(Y|X_1)$, where $Y \sim p(y|X_1)$. The we obtain

$$e_{ABE} = \Pr[Z_1 < \max_{j>1} Z_i].$$

Our proof uses the assumption that $Z_1, \ldots, Z_k$ are asymptotically multivariate normal. Supposing that $Z_1, \ldots, Z_k$ are indeed asymptotically normal, the following lemma allows us to obtain a formula for the misclassification rate.

Lemma 1. *Suppose $(Z_1, Z_2, \ldots, Z_k)$ are jointly multivariate normal, with $\boldsymbol{E}[Z_1 - Z_i] = \alpha$, $Var(Z_1) = \beta$, $Cov(Z_1, Z_i) = \gamma$, $Var(Z_i) = \delta$, and $Cov(Z_i, Z_j) = \epsilon$ for all $i, j = 2, \ldots, k$, such that $\beta + \epsilon - 2\gamma > 0$. Then, letting*

$$\mu = \frac{\boldsymbol{E}[Z_1 - Z_i]}{\sqrt{\frac{1}{2} Var(Z_i - Z_j)}} = \frac{\alpha}{\sqrt{\delta - \epsilon}},$$

$$\nu^2 = \frac{Cov(Z_1 - Z_i, Z_1 - Z_j)}{\frac{1}{2} Var(Z_i - Z_j)} = \frac{\beta + \epsilon - 2\gamma}{\delta - \epsilon},$$

we have

$$\begin{aligned} \Pr[Z_1 < \max_{i=2}^{k} Z_i] &= \Pr[W < M_{k-1}] \\ &= 1 - \int \frac{1}{\sqrt{2\pi\nu^2}} e^{-\frac{(w-\mu)^2}{2\nu^2}} \Phi(w)^{k-1} dw, \end{aligned}$$

where $W \sim N(\mu, \nu^2)$ and M_{k-1} is the maximum of $k-1$ independent standard normal variates, which are independent of W.

[[proof in appendix]]

To see why the assumption that $Z_1, \ldots, Z_k$ are multivariate normal might be justified, suppose that X and Y have the same dimensionality d, and that joint density factorizes as

$$p(x_j, y) = \prod_{i=1}^{d} p_i(x_{j,i}, y_i)$$

where $x_{j,i}, y_i$ are the components of x_j and y. Then,

$$Z_i = \sum_{m=1}^{d} \log p_m(y_m|x_{m,i}) - \log p_m(y_m|x_{m,1})$$

where $x_{i,j}$ is the ith component of x_j. The d terms $\log p_m(y_m|x_{m,i}) - \log p_m(y_m|x_{m,1})$ are independent across the indices m, but dependent between the $i = 1, \ldots, k$. Therefore, the multivariate central limit theorem can be applied to conclude that the vector $(Z_1, \ldots, Z_k)$ can be scaled to converge to a multivariate normal distribution. Now, since the average Bayes error $e_{ABE,k}$ is a continuous functional of the joint distribution $p(x, y)$, it follows that $e_{ABE,k}$ converges to a functional of the limiting mean and covariance of $(Z_1, \ldots, Z_k)$, assuming that the limits exist. In our theorem, we assume a specific regime where these limits exist as a consequence. While the componentwise independence condition is not a realistic assumption, the key property of multivariate normality of $(Z_1, \ldots, Z_k)$ holds under more general conditions, and appears reasonable in practice.

The second component of our theorem is to manipulate the expression of the mutual information $I(X; Y)$. The differential mutual information is defined as

$$I(X; Y) = \int p(x, y) \log \frac{p(x, y)}{p(x)p(y)} dxdy.$$

The key manipulation we employ is to approximate the logarithmic term by the Taylor expansion

$$\log \frac{p(x, y)}{p(x)p(y)} \approx \frac{p(x, y) - p(x)p(y)}{p(x)p(y)} - \left(\frac{p(x, y) - p(x)p(y)}{p(x)p(y)} \right)^2 + \ldots.$$

The approximation is accurate if $I(X; Y)$ is small–or rather, small relative to the dimensionality within the asymptotic sequence. We state the theorem for the regime where $I(X; Y)$ is fixed, while the dimensionality of X increases.

The asymptotic regime we consider is one where the dimension of X goes to infinity. This means that we have to consider a sequence of joint distributions $(X^{[d]}, Y^{[d]})$ indexed by the dimension d.

Fix integer $k \geq 2$. Let $p^{[d]}(x, y)$ be a sequence of probability density functions, where x is of dimension $p^{[d]}$ and y is of dimension $q^{[d]}$. Let $p^{[d]}(x)$ and $p^{[d]}(y)$ denote the marginal densities, and let

$$p^{[d]}(y|x) = p^{[d]}(x, y)/p^{[d]}(y).$$

Let $(X^{([d],i)}, Y^{([d],i)})$ be iid random variates from $p^{[d]}(x, y)$ for $i = 1, \ldots, k$; we will supress the superscripts $[d]$ and/or (i) when convenient. Recall the definitions of entropy,

$$H(X) = -\int p(x) \log p(x) dx,$$

and mutual information

$$I(X; Y) = \int p(x, y) \log \frac{p(x, y)}{p(x)p(y)} dxdy.$$

Furthermore, define the K-class average Bayes error as

$$e_{ABE,k} = \Pr[p(Y^{(1)}|X^{(1)}) < \max_{i=2}^{k} p(Y^{(1)}|X^{(i)})].$$

Define

$$u^{[d]}(x, y) = \log p^{[d]}(x, y) - \log p^{[d]}(x) - \log p^{[d]}(y),$$

and define

$$\ell_{ij}^{[d]} = \log p(y^{(i)}|x^{(j)}).$$

We now give the theorem and its proof.

Theorem 1. Let $p^{[d]}(x, y)$ be a sequence of joint densities for $d = 1, 2, \ldots$ as given above. Further assume that

A1. $\lim_{d\to\infty} I(X^{[d]}; Y^{[d]}) = \iota < \infty$.

A2. There exists a sequence of scaling constants $a_{ij}^{[d]}$ and $b_{ij}^{[d]}$ such that the random vector $(a_{ij}\ell_{ij}^{[d]} + b_{ij}^{[d]})_{i,j=1,\ldots,k}$ converges in distribution to a multivariate normal distribution.

A3. There exists a sequence of scaling constants $a^{[d]}$, $b^{[d]}$ such that

$$a^{[d]}u(X^{(1)}, Y^{(2)}) + b^{[d]}$$

converges in distribution to a univariate normal distribution.

A4. For all $i \neq k$,

$$\lim_{d\to\infty} \text{Cov}[u(X^{(i)}, Y^{(j)}), u(X^{(k)}, Y^{(j)})] = 0.$$

Then for $e_{ABE,k}$ as defined above, we have

$$\lim_{d\to\infty} e_{ABE,k} = \pi_k(\sqrt{2\iota})$$

where

$$\pi_k(c) = 1 - \int_{\mathbb{R}} \phi(z - c)\Phi(z)^{k-1}dz$$

where ϕ and Φ are the standard normal density function and cumulative distribution function, respectively.

[Proof in supplemtn]

Assumptions A1-A4 are satisfied in a variety of natural models. One example is a multivariate Gaussian sequence model where

$$X \sim N(0, \Sigma_d)$$
$$E \sim N(0, \Sigma_e)$$
$$Y = X + E$$

where Σ_d and Σ_e are $d \times d$ covariance matrices, and where X and E are independent. Then, if $d\Sigma_d$ and Σ_e have limiting spectra H and G respectively, the joint densities $p(x, y)$ for $d = 1, \ldots,$ satisfy assumptions A1 - A4.

We can also construct a family of densities satisfying A1 - A4, which we call an *exponential family sequence model* since each joint distribution in the sequence is a member of an exponential family: details are given in the supplement. One example of such an exponential family sequence model is a multivariate logistic regression model, given by

$$X \sim N(0, I)$$

$$Y_i \sim \text{Bernoulli}(e^{\beta X_i}/(1 + e^{\beta X_i}))$$

The multivariate logistic regression model (and multivariate Poisson regression model) are especially suitable for modeling neural spike count data; we simulate data from such a multivariate logistic regression model in section X.

Since π_k is invertible for all $k = 2, \ldots$, a converse relationship

$$\lim_{d\to\infty} I(X^{[d]}; Y^{[d]}) = \frac{1}{2}(\pi_k^{-1}(\eta))^2$$

also holds in the same regime. We formally state the result, and a few consequences, as follows.

Corollary 1. Let $p^{[d]}(x, y)$ be a sequence of joint densities for $d = 1, 2, \ldots$ as given above. Further assume assumptions A2 - A4 and also

A1'. $\lim_{d\to\infty} e_{ABE,k} = \eta < \infty$.

Then

i.
$$\lim_{d\to\infty} I(X^{[d]}; Y^{[d]}) = \frac{1}{2}(\pi_k^{-1}(e_{ABE}))^2.$$

ii. If $[\underline{e}, \bar{e}]$ is a $1-\alpha$ confidence interval for $e_{ABE,k}$, then
$$[\frac{1}{2}(\pi_k^{-1}(\bar{e}))^2, \frac{1}{2}(\pi_k^{-1}(\underline{e}))^2]$$
is asymptotically a $1-\alpha$ confidence interval of $I(X;Y)$: that is,
$$\lim_{d\to\infty} \Pr\left[I(X^{[d]}; Y^{[d]}) \in [\frac{1}{2}(\pi_k^{-1}(\underline{e}))^2, \frac{1}{2}(\pi_k^{-1}(\bar{e}))^2]\right] = 1-\alpha.$$

iii. If $\hat{e}$ is a $O(1/\sqrt{n})$-consistent estimator for $e_{ABE,k}$, and $\lim_{d\to\infty} e_{ABE,k} > 0$, then $\frac{1}{2}(\pi_k^{-1}(\hat{e}))^2$ is a $O(1/\sqrt{n})$-consistent estimator for $I(X;Y)$.

[[Proof in appendix]]

As corollary 1 states, it is possible to construct a confidence interval for $I(X;Y)$ by first constructing a confidence interval for the average Bayes error $e_{ABE,k}$; then obtaining the confidence interval for $I(X;Y)$ as
$$[\frac{1}{2}(\pi_k^{-1}(\bar{e}))^2, \frac{1}{2}(\pi_k^{-1}(\underline{e}))^2].$$

Corollary 1 also gives the consisistent point estimate
$$\hat{I}(X;Y) = \frac{1}{2}(\pi_k^{-1}(\hat{e}))^2,$$
where $\hat{e}$ is a $O(1/\sqrt{n})$-consistent estimate of $e_{ABE,k}$. However, $\hat{I}(X,Y)$ may perform poorly in finite samples due to bias. Better performance can be obtained by using bias-correction and shrinkage, but the optimality of the estimator depends on the choice of risk function and risk criterion. In the remainder of the paper, we will be mainly interested in interval estimation.

3 Results

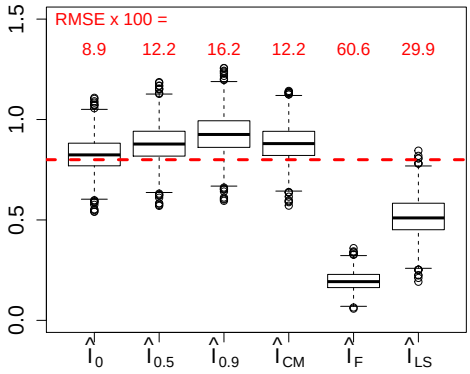
Multiple-response logistic regression model
$$X \sim N(0, I_p)$$
$$Y \in \{0,1\}^q$$
$$Y_i|X = x \sim \text{Bernoulli}(x^T B_i)$$
where B is a $p \times q$ matrix.

Methods.

- Nonparametric: $\hat{I}_0$ naive estimator, $\hat{I}_\alpha$ anthropic correction.
- ML-based: $\hat{I}_{CM}$ confusion matrix, $\hat{I}_F$ Fano, $\hat{I}_{LS}$ low-SNR method.

Sampling distribution of $\hat{I}$ for $\{p = 3, B = \frac{4}{\sqrt{3}} I_3, K = 20, r = 40\}$.

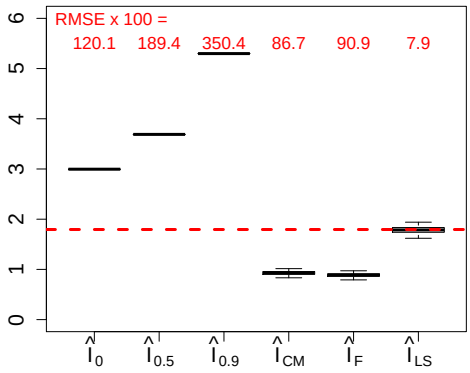
True parameter $I(X;Y) = 0.800$ *(dotted line.)*



Naïve estimator performs best! $\hat{I}_{LS}$ not effective.

Sampling distribution of $\hat{I}$ for $\{p = 50,\ B = \frac{4}{\sqrt{50}} I_{50},\ K = 20,\ r = 8000\}$.

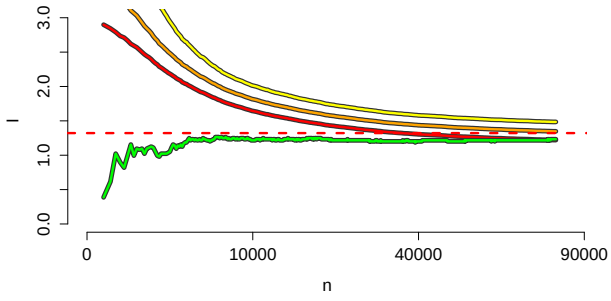
True parameter $I(X;Y) = 1.794$ *(dashed line.)*



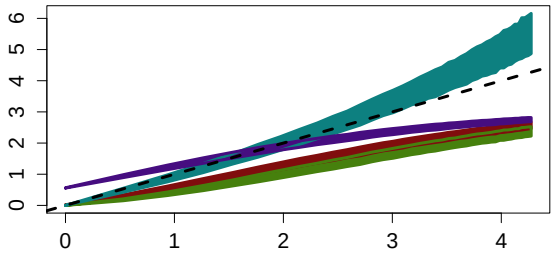
Non-parametric methods extremely biased.

Estimation path of $\hat{I}_{LS}$ and $\hat{I}_\alpha$ as n ranges from 10 to 8000.

$\{p = 10,\ B = \frac{4}{\sqrt{10}} I_{10},\ K = 20\}$. True parameter $I(X;Y) = 1.322$ *(dashed line.)*



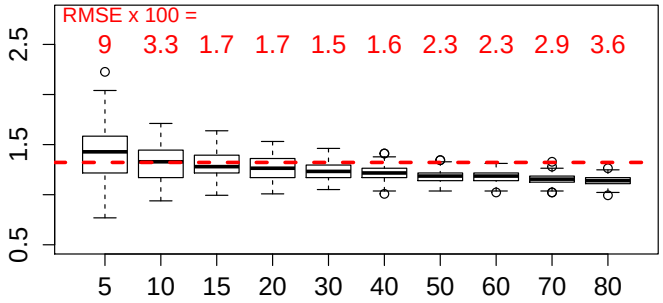
Estimated $\hat{I}$ vs true I.



Sampling distribution of $\hat{I}_{LS}$ for $\{p = 10, B = \frac{4}{\sqrt{10}} I_{10}, N = 80000\}$,

and $K = \{5, 10, 15, 20, \ldots, 80\}$, $r = N/k$.

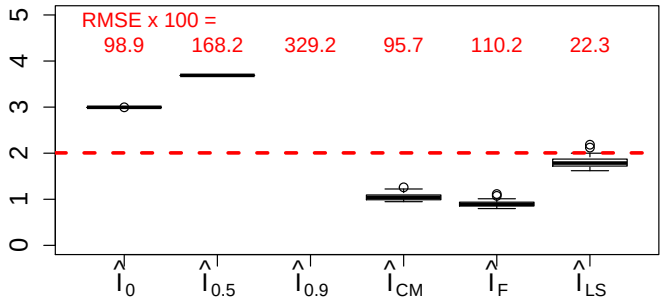
True parameter $I(X;Y) = 1.322$ *(dashed line.)*



Decreasing variance as K increases. Bias at large and small K.

$p = 20$ and $q = 40$, entries of B are iid $N(0, 0.025)$.

$K = 20$, $r = 8000$, true $I(X;Y) = 1.86$ *(dashed line.)*



Sampling distribution of $\hat{I}$.

4 Discussion

Acknowledgments

Use unnumbered third level headings for the acknowledgments. All acknowledgments go at the end of the paper. Do not include acknowledgments in the anonymized submission, only in the final paper.

References

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