Estimating mutual information in high dimensions via 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 assumption or prior. One approach is to assume a parametric joint distribution on (X, Y), but in many applications, such a strong modeling assumption cannot be justified. Alternatively, one can estimate the mutual information based the performance of a classifier trained on the data. Existing methods include using the empirical mutual information of the confusion matrix of the classifier, as well as an estimator based on Fano's inequality. However, both of these methods all produce an estimate which is bounded by $\log(k)$, where k is the number of classes. This presents a substantial limitation for classification-based approaches, since the number of repeats per class must be large for the classifier to work well, hence limiting the number of classes k that can be defined. In this paper, we construct a novel classification-based estimator of mutual information which overcomes these limitations. Our estimator is based on high-dimensional asymptotics: we show that in a particular limiting regime, the mutual information is an invertible function of the expected k-class Bayes error. While the theory is based on a large-sample, high-dimensional limit, we demonstrate through simulations that our proposed estimator 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 [1], to quantifying the information between a random stimulus X and the signaling behavior of an ensembles of neurons, Y [2]; for use as an objective function for training neural networks [3], for feature selection in machine learning, and even as an all-purpose nonlinear measure of "correlation for the 21st century" [4]. 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, see [5] for a review.

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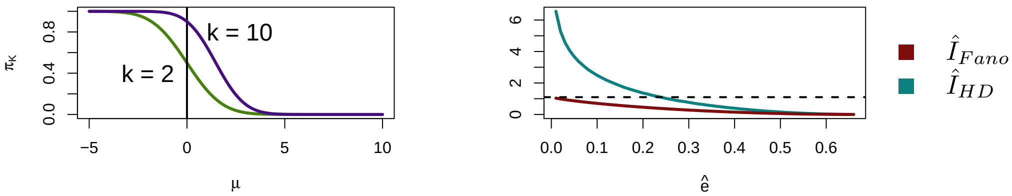

Figure 1: Left: The function $pi_k(\mu)$ for $k = \{2, 10\}$. Right: $\hat{I}_{HD}$ with $\hat{I}_{Fano}$ as functions of $\hat{e}_{gen}$, for $k = 3$. While $\hat{I}_{Fano}$ is bounded from above by $\log(k)$ (dotted line), $\hat{I}_{HD}$ is unbounded.

However, the sample complexity for nonparametric estimation grows exponentially with the dimension, rendering such methods ineffective in applications with high-dimensional data [5]. One such application includes multivariate pattern analysis (MVPA), an area of neuroscience research pioneered by Haxby [6], 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 [7] 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 [8]. 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. Therefore, one can construct an estimator based on Fano's inequality, $\hat{I}_{Fano}$. In either case, any method which derives an estimate of mutual information from classification performance may be considered a *discriminative* estimation procedure, in contrast to the *parametric* and *nonparametric* classes of estimation procedures.

We derive a new discriminative estimator by exploiting an assumption on the random sampling of the classes (described in section 1.1) and also a universality property that arises in high-dimensions. This universality phenomenon allows us 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),

$$e_{ABE,k} \approx \pi_k(\sqrt{2I(X;Y)}) \tag{1}$$

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. The function π_k is given by

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

This formula is not new to the information theory literature: it appears as the error rate of an orthogonal constellation [13]. What is surprising is that the same formula can be used to approximate the error rate in much more general class of classification problems[1]–this is precisely the universality result which provides the basis for our proposed estimator.

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 $\mu \to \infty$, which is what we expect since if $I(X; Y)$ is large, then the average Bayes error should be small. Another intuitive fact is that $\pi_k(0) = 1 - \frac{1}{k}$, since after all, an uninformative response cannot lead to above-chance classification accuracy.

[1] An intuitive explanation for this fact is that points from any high-dimensional distribution lie in an orthogonal configuration with high probability.

In this paper, we argue for the advantages of our method in comparison to alternative discriminative estimators under the assumption that the discriminative model approximates the Bayes rule. While this is an unrealistic assumption, it simplifies the theoretical discussion, and allows us to clearly discuss the principles behind our method. We outline our framework in the following section.

1.1 Setting

Let us 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 assume that data is collected using *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 $F_{X^{(Z_i)}}$.

Stratified sampling is 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. [2]

When stratified sampling is employed, one can define an *exemplar-based* classification task. One defines the *class function* Z by

$$Z : \{X^{(1)}, \ldots, X^{(k)}\} \to \{1, \ldots, k\},$$
$$Z(X^{(i)}) = i \text{ for } i = 1, \ldots, k.$$

One defines the generalization error by

$$e_{gen}(f) = \frac{1}{k}\sum_{i=1}^{k} \Pr[f(Y) \neq Z | X = X^{(i)}]. \tag{2}$$

In an exemplar-based classification, there is no need to specify an arbitrary partition on the input space (as is the case in category-based classification), but now 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. Therefore, it is useful to consider the *average Bayes error*,

$$e_{ABE,k} = \mathbf{E}_{X^{(1)},\ldots,X^{(k)}}[e_{Bayes}], \tag{3}$$

where the expectation is taken over the joint distribution of $X^{(1)}, \ldots, X^{(k)} \stackrel{iid}{\sim} G$.

Unless expert knowledge is available, it is usually necessary to choose the function f in a data-dependent way in order to obtain a reasonable classification rule. We use the terminology *classifier* to refer to any algorithm which takes data as input, and produces a classification rule f as output. 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 goal is to obtain *inference* about the generalization error e_{gen} of the classification rule f, it becomes 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 [10]. One creates a *training set* consisting of r_1 repeats per class, $S_{train} = \{(x^{(i)}, y^{(i),j})\}_{i=1,j=1}^{k,r_1}$, and a *test set* consisting of the remaining $r_2 = r - r_1$ repeats, $S_{test} = \{(x^{(i)}, y^{(i),j})\}_{i=1,j=r_1}^{k,r}$. The classification rule is obtained via $f = \mathcal{F}(S_{train})$, and the performance of the classifier is evaluated by predicting the classes of the test set. The results of this test are summarized by a $k \times k$ *confusion matrix* M with $M_{ij} = \sum_{\ell=r_1+1}^{r} I(f(y^{(i),r}) = j)$. The i, jth entry of M counts how many times a output in the ith class was classified to the jth class. The *test error* is the proportion of off-diagonal terms of M, $e_{test} = \frac{1}{kr}\sum_{i\neq j} M_{ij}$, and is an unbiased estimator of e_{gen}. However, in small sampling regimes the quantity e_{test} may be too variable to use

[2]Note the asymmetry in our definition of stratified sampling: our convention is to take X to be the variable preceding Y in causal order. Such causal directionality constrains the stratified sampling to have repeated X rather than repeated Y values, but has no consequence for the mutual information $I(X; Y)$, which is a symmetric function.

as an estimator of e_{gen}. We recommend the use of Bayesian smoothing, defining an α-smoothed estimate $\hat{e}_{gen,\alpha}$ by $\hat{e}_{gen,\alpha} = (1-\alpha)e_{test} + \alpha\frac{k-1}{k}$, which takes a weighted average of the unbiased estimate e_{test}, and the natural prior of *chance classification*.

We define a discriminative estimator to be a function which maps the misclassification matrix to a positive number, $\hat{I} : \mathbb{N}^{k\times k} \to \mathbb{R}$. We are aware of the following examples of discriminative estimators: (1) estimators $\hat{I}_{Fano}$ derived from using Fano's inequality, and (2) the empirical information of the confusion matrix, $\hat{I}_{CM}$, as introduced by Treves [7]. We discuss these estimators in section 3.

In section 2 we present an asymptotic setting intended to capture the notion of high dimensionality; namely, one where the number of classes is fixed, and where the information $I(X;Y)$ remains fixed, while the dimensionality of the input X and output Y both grow to infinity. We make a number of additional regularity conditions to rule out scenarios where (X,Y) is really less "high-dimensional" than it appears, since most of the variation is captured a low-dimensional manifold[3]. In section 2.1 we present our key result, which links the asymptotic average Bayes error to the mutual information; in section 2.2 we apply this result to derive our proposed estimator, $\hat{I}_{HD}$ (where HD stands for "high-dimensional.") Section 3 presents simulation results, and section 4 concludes. All proofs are given in the supplement.

2 Theory

2.1 Universality result

We obtain the universality result in two steps. First, we link the average Bayes error to the moments of some statistics Z_i. Secondly, we use taylor approximation in order to express $I(X;Y)$ in terms of the moments of Z_i. Connecting these two pieces yields the formula (1).

Let us start by rewriting the average Bayes error:

$$e_{ABE,k} = \Pr[p(Y|X_1) \leq \max_{j\neq 1} p(Y|X_j)|X = X_1].$$

Defining the statistic $Z_i = \log p(Y|X_i) - \log p(Y|X_1)$, where $Y \sim p(y|X_1)$, we obtain $e_{ABE} = \Pr[\max_{j>1} Z_i > 0]$. The key assumption we need is that $Z_2,\ldots,Z_k$ are asymptotically multivariate normal. If so, 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$(Z_1) = \beta \geq 0$, 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

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

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.

To see why the assumption that $Z_2,\ldots,Z_k$ are multivariate normal might be justified, suppose that X and Y have the same dimensionality d, and that joint density factorizes as

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

[3]In situations where (X,Y) lie on a manifold, one could effectively estimate mutual information by would be to combining dimensionality reduction with nonparametric information estimation [12].

where $x_i^{(j)}, y_i$ are the ith scalar components of the vectors $x^{(j)}$ and y. Then,

$$Z_i = \sum_{m=1}^{d} \log p_m(y_m|x_m^{(i)}) - \log p_m(y_m|x_1^{(m)})$$

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 $(Z_2, \ldots, Z_k)$ can be scaled to converge to a multivariate normal distribution. While the componentwise independence condition is not a realistic assumption, the key property of multivariate normality of $(Z_2, \ldots, Z_k)$ holds under more general conditions, and appears reasonable in practice.

It remains to link the moments of Z_i to $I(X;Y)$. This is accomplished by approximating the logarithmic term by the Taylor expansion

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

A number of assumptions are needed to ensure that needed approximations are sufficiently accurate; and additionally, in order to apply the central limit theorem, we need to consider a *limiting sequence* of problems with increasing dimensionality. We now state the theorem.

Theorem 1. *Let $p^{[d]}(x,y)$ be a sequence of joint densities for $d = 1, 2, \ldots$. 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. Define

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

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

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

converges in distribution to a univariate normal distribution.

A4. For all $i \neq k$,

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

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.

Assumptions A1-A4 are satisfied in a variety of natural models. One example is a multivariate Gaussian sequence model where $X \sim N(0, \Sigma_d)$ and $Y = X + E$ with $E \sim N(0, \Sigma_e)$, 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. Another example is the multivariate logistic model, which we describe in section 3. We further discuss the rationale behind A1-A4 in the supplement, along with the detailed proof.

2.2 High-dimensional estimator

The estimator we propose is

$$\hat{I}_{HD}(M) = \frac{1}{2}(\pi_k^{-1}(\hat{e}_{gen,\alpha}))^2,$$

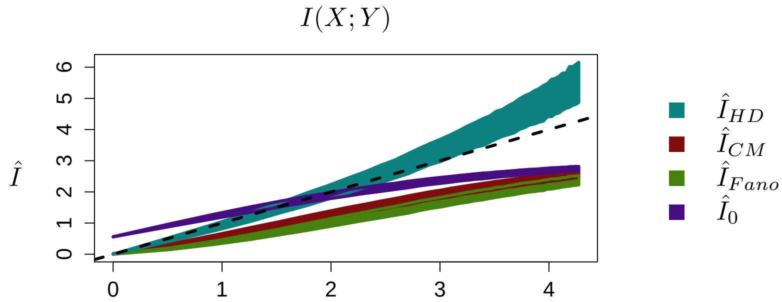

Figure 2: Sampling distributions of $\hat{I}$ for data generated from the multiple-response logistic model. $p = q = 10$; $k = 20$; $B = sI_{10}$, where $s \in [0, \sqrt{200}]$; and $r = 1000$.

obtained by inverting the relation (1), then substituting the estimate $\hat{e}_{gen,\alpha}$ for the $e_{ABE,k}$. As such, our estimator can be directly compared to the $\hat{I}_{Fano}$, since both are functions of $\hat{e}_{gen,\alpha}$ (Figure 1.)

For sufficiently high-dimensional problems, $\hat{I}_{HD}$ can accurately recover $I(X;Y) > \log k$, supposing also that the classifier $\mathcal{F}$ consistently estimates the Bayes rule. The number of observations needed depends on the convergence rate of $\mathcal{F}$ and also the complexity of estimating $e_{gen,\alpha}$. Therefore, without making assumptions on $\mathcal{F}$, the sample complexity is at least exponential in $I(X;Y)$. This is because when $I(X;Y)$ is large relative to $\log(k)$, the Bayes error $e_{ABE,k}$ is exponentially small. Hence $O(1/e_{ABE,k})$ observations in the test set are needed to recover $e_{ABE,k}$ to sufficient precision. While the sample complexity exponential in $I(X;Y)$ is by no means ideal, by comparison, the nonparametric estimation approaches have a complexity exponential in the dimensionality. Hence, $\hat{I}_{HD}$ is favored over nonparametric approaches in settings with high dimensionality and low signal-to-noise ratio.

3 Simulation

We compare the discriminative estimators $\hat{I}_{CM}$, $\hat{I}_{Fano}$, $\hat{I}_{HD}$ with a nonparametric estimator $\hat{I}_0$ in the following simulation. We generate data according to a multiple-response logistic regression model, where $X \sim N(0, I_p)$, and Y is a binary vector with conditional distribution

$$Y_i | X = x \sim \text{Bernoulli}(x^T B_i)$$

where B is a $p \times q$ matrix. One application of this model might be modeling neural spike count data Y arising in response to environmental stimuli X [14]. We choose the naive Bayes for the classifier $\mathcal{F}$: it is consistent for estimating the Bayes rule.

The estimator $\hat{I}_{Fano}$ is based on Fano's inequality, which reads

$$H(Z|Y) \leq H(e_{Bayes}) + e_{Bayes} \log ||\mathcal{Z}| - 1|$$

where $H(e)$ is the entropy of a Bernoulli random variable with probability e. Replacing $H(Z|Y)$ with $H(X|Y)$ and replacing e_{Bayes} with $\hat{e}_{gen,\alpha}$, we get the estimator

$$\hat{I}_{Fano}(M) = log(K) - \hat{e}_{gen,\alpha} log(K-1) + \hat{e}_{gen,\alpha} log(p) + (1 - \hat{e}_{gen,\alpha}) log(1 - \hat{e}_{gen,\alpha}).$$

Meanwhile, the confusion matrix estimator computes

$$\hat{I}_{CM}(M) = \frac{1}{k^2} \sum_{i=1}^{k} \sum_{j=1}^{k} \log \frac{M_{ij}}{r/k},$$

which is the empirical mutual information of the discrete joint distribution $(Z, f(Y))$.

It is known that $\hat{I}_{CM}$, $\hat{I}_0$ tend to underestimate the mutual information. Quiroga et al. [8] discussed two sources of 'information loss' which lead to $\hat{I}_{CM}$ underestimating the mutual information: the discretization of the classes, and the error in approximating the Bayes rule. Meanwhile, Gastpar et al. [11] showed that $\hat{I}_0$ is biased downwards due to undersampling of the exemplars: to counteract this bias, they introduce the anthropic correction estimator $\hat{I}_\alpha$[4].

In addition to the sources of information loss discussed by Quiroga et al., an additional reason why $\hat{I}_{CM}$ and $\hat{I}_{Fano}$ underestimate the mutual information is that they are upper bounded by $\log(k)$, where k is the number of classes. As $I(X;Y)$ exceeds $\log(k)$, the estimate $\hat{I}$ can no longer approximate $I(X;Y)$, even up to a constant factor. In contrast, $\hat{I}_{HD}$ is unbounded and may either underestimate or overestimate the mutual information in general, but performs well when the high-dimensionality assumption is met.

In Figure 2 we show the sampling distributions of the four estimators as $I(X;Y)$ is varied in the interval $[0,4]$. We see that $\hat{I}_{CM}$, $\hat{I}_{Fano}$, and $\hat{I}_0$ indeed begin to asymptote as they approach $\log(k) = 2.995$. In contrast, $\hat{I}_{HD}$ remains a good approximation of $I(X;Y)$ within the range, although it begins to overestimate at the right endpoint. The reason why $\hat{I}_{HD}$ loses accuracy as the true information $I(X;Y)$ increases is that the multivariate normality approximation used to derive the estimator becomes less accurate when the conditional distribution $p(y|x)$ becomes highly concentrated.

4 Discussion

Discriminative estimators of mutual information have the potential to estimate mutual information in high-dimensional data without resorting to fully parametric assumptions. However, a number of practical considerations also limit their usage. First, one has to find a good classifier $\mathcal{F}$ for the data: techniques for model selection can be used to choose $\mathcal{F}$ from a large library of methods. However, there is no way to guarantee how well the chosen classifier approximates the optimal classification rule. Secondly, one has to estimate the generalization error from test data: the complexity of estimating e_{gen} could become the bottleneck when e_{gen} is close to 0. Thirdly, for previous estimators $\hat{I}_{Fano}$ and $\hat{I}_{CM}$, the ability of the estimator to distinguish high values of $I(X;Y)$ is limited by the number of classes k. Our estimator $\hat{I}_{HD}$ is subject to the first two limitations, along with any conceivable discriminative estimator, but overcomes the third limitation under the assumption of stratified sampling and high dimensionality.

It can be seen that additional assumptions are indeed needed to overcome the third limitation, the $\log(k)$ upper bound. Consider the following worst-case example: let X and Y have joint density $p(x,y) = \frac{1}{k} I(\lfloor kx \rfloor = \lfloor ky \rfloor)$ on the unit square. Under partition-based classification, if we set $Z(x) = \lfloor kx \rfloor + 1$, then no errors are made under the Bayes rule. We therefore have a joint distribution which maximizes any reasonable discriminative estimator but has *finite* information $I(X;Y) = \log(k)$. The consequence of this is that under partition-based classification, we cannot hope to distinguish distributions with $I(X;Y) > \log(k)$. The situation is more promising if we specialize to stratified sampling: in the same example, a Bayes of zero is no longer likely due to the possibility of exemplars being sampled from the same bin ('collisions')–we obtain an approximation to the average Bayes error through a Poisson sampling model: $e_{ABE,k} \approx \frac{1}{e} \sum_{j=1}^{\infty} \frac{1}{j(j!)} = 0.484$. By specializing further to the high-dimensional regime, we obtain even tighter control on the relation between Bayes error and mutual information. Our estimator therefore provides more accurate estimation at the cost of more additional assumptions, but just how restrictive are these assumptions?

The assumption of stratified sampling is usually not met in the most common applications of classification where the classes are defined *a priori*. For instance, if the classes consist of three different species of iris, it does not seem appropriate to model the three species as i.i.d. draws from some distribution on a space of infinitely many potential iris species. Yet, when the classes have been pre-defined in an arbitrary manner, the mutual information between a latent class-defining variable X and Y may be only weakly related to the classification accuracy. We rely on the stratified sampling assumption to obtain the necessary control on how the classes in the classification task are defined. Fortunately, in many applications where one is interested in estimating $I(X;Y)$, a stratified sampling design can be practically implemented.

[4] However, without a principled approach to choose the parameter $\alpha \in (0,1]$, $\hat{I}_\alpha$ could still vastly underestimate or overestimate the mutual information.

The assumption of high dimensionality is not easy to check: having a high-dimension response Y does not suffice, since Y could lie close to a low-dimensional manifold. In such cases, $\hat{I}_{HD}$ could either overestimate or underestimate the mutual information. One useful diagnostic is to subsample within the classes collected and check that $\hat{I}_{HD}$ does not systematically increase or decrease with the number of classes k.

The assumption of approximating the Bayes rule is impractical to check, as any nonparametric estimate of the Bayes error requires exponentially many observations. Hence, while the present paper studies the 'best-case' scenario where the model is well-specified, it is even more important to understand the robustness of our method in the more realistic case where the model is misspecified. We leave this question to future work.

All of these three assumptions are met in our simulation experiment, hence our proposed estimator is seen to dramatically outperform existing estimators. It remains to assess the utility of our estimation procedure in a real-world example, where both the high-dimensional assumption and the model specification assumption are likely to be violated. In a forthcoming work, we apply our framework to evaluate visual encoding models in human fMRI data.

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