Bootstrap Estimation of a Non-Parametric Information Divergence Measure

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Abstract

This work details the bootstrap estimation of a nonparametric information divergence measure, the D_p divergence measure, applied to the binary classification problem. To address the challenge posed by computing accurate divergence estimates given finite size data, the bootstrap approach is used in conjunction with a power law curve to calculate an asymptotic value of the divergence measure estimate. Monte Carlo estimates of D_p are found for increasing values of sample data size, and a power law fit is used to find the asymptotic value of the divergence measure as a function of sample size. The fit is also used to generate a confidence interval for the estimate to characterize the quality of the estimator, and the result obtained for the divergence measure is then compared to the result using other resampling methods. Using the inherent relation between divergence measures and classification error rate, an analysis of the Bayes error rate of several test data sets is conducted via this power law estimation approach for D_p.

1 Introduction

Information divergence measures have a wide variety of applications in machine learning, pattern recognition, feature extraction, and big data analysis [8]. The two main classes of information divergence measures are parametric and nonparametric measures. Nonparametric divergence measures, notably including f-divergences such as the Kullback-Leibler (KL) divergence, measure the difference between two distributions F_0 and F_1. Arguably the most well known f-divergence, the KL Divergence is a measure of relative entropy and has applications in coding theory, feature selection, and hypothesis testing [20]. Given these wide variety of applications, there is great interest in estimation of f-divergences.

Normally, when estimating the divergence between two distributions, we have access to independent and identically distributed (i.i.d) training data from each distribution $X_i \in c_0$ and $Y_i \in c_1$ (where c_0, c_1 correspond to two classes of data). The challenge in estimating the divergence measure between two datasets is that the distributions of the data F_0 and F_1 are usually unknown. An f-divergence, D_ϕ, is of the form:

$$D_\phi(F_0, F_1) = \int_\Omega \phi\left(\frac{dF_0}{dF_1}\right) dF_0 \tag{1}$$

given a convex function $\phi(x)$, and feature space Ω [20]. As we lack knowledge of the distribution functions F_0 and F_1, a direct computation of D_ϕ is not possible.

A naive method to calculate the divergence between the data is to first find the densities for X_i and Y_i, and then calculate the divergence from the computed density estimates. However, as noted in [5] density estimation adds an undesirable intermediate step before the computation of the divergence measure, introduces additional error, and can be difficult for cases of high dimensionality.

In this paper, we perform a bootstrap estimation of a minimum spanning tree based f-divergence derived in [25] using a power law. From data of size N, we compute Monte Carlo iterations at i sample sizes $n \in \{n_1, n_2, \dots, n_i\} < N$, and apply the unproven, but reasonable assumption that a power law fit can be used to characterize the divergence estimator as a function of sample size. We exploit the unique ability to estimate this divergence measure directly from data, and bypass computing the densities. Utilizing this curve we extrapolate as sample size $n \to \infty$, and find the asymptotic value of the divergence estimate from a finite length data set. As f-divergences are related to the classification error rate [19], this estimation scheme is applied to binary classification examples to find Bayes error rates for several datasets.

The work is organized as follows: the remainder of Section 1 is devoted to background and previous work. Section 1.1-1.2 discusses f-divergences, their connection to the Bayes optimal error rate, and introduce the specific divergence measure used. Section 1.3 discusses the motivation for the bootstrap power law estimation method, which is formally described in Section 2. In Section 3, examples of the estimation approach are given. In 3.1 we consider generated datasets with known divergence values to demonstrate the accuracy of the estimation algorithm. In 3.2 we perform analysis on the Pima Indians data set and the Banknote data set and compare the calculated Bayes error rates to the classification error rates reported in the literature.

Background and Previous Work

1.1 Divergences Measures

1.1.1 f-divergences

From equation (1), it is clear that f-divergences are a function of the distributions of the data from each class. In terms of the probability densities $f_0(x)$ and $f_1(x)$, the equation may be rewritten as follows:

$$D_f(f_0, f_1) = \int_\Omega f\left(\frac{f_0(\mathbf{x})}{f_1(\mathbf{x})}\right) f_1(\mathbf{x}) dx \tag{2}$$

The resultant divergence is dependent on the choice of $f(x)$. For example, the K-L divergence corresponds to $f(x) = -ln(x)$ [6]. A table of commonly used divergences is given below.

Table 1: Commonly Used f-Divergences

Divergence Measure	D_f
K-L Divergence	$\int f_1(x) ln(\frac{f_0(x)}{f_1(x)}) dx$
L^2 Divergence	$\int (f_0(x) - f_1(x))^2 dx$
Total Variation Distance	$\frac{1}{2} \int \lvert f_0(x) - f_1(x) \rvert dx$
Bhattacharya Distance	$\int \sqrt{f_0(x) f_1(x)} dx$

Note that for some cases the divergence may yield values that are not bounded depending on the choice of $f(x)$.

Since in most cases, direct evaluation of the integrals is not possible due to unknown densities, a number of estimation methods have been used to make the problem more tractable. Wang *et al.* [27] derived a nonparametric divergence estimator based on estimating the density ratio $\frac{dF_0}{dF_1}$, and in [28] defined a k-Nearest-Neighbors based divergence estimator that also requires a density ratio estimate. But, calculation of $\frac{dF_0}{dF_1}$ rather than $f_0(\mathbf{x})$ and $f_1(\mathbf{x})$ still poses the same drawback: it is undesirable to estimate the divergence by performing the intermediate step of estimating a quantity related to the probability distributions.

A key advantage of the f-divergence we consider is that it can be estimated from the data samples themselves, without intermediate density estimation steps. Towards this end, Hero *et al.* derive a divergence estimator assuming one of the distributions was known. Póczos *et al.* [29] derive estimators for Rényi and L_2 divergences based on k-Nearest Neighbors statistics, and apply the estimate for classifying astronomical data. We consider the f-divergence described in [25], which enables nonparametric divergence estimation directly from sample data via generating a Euclidean minimum spanning tree (MST).

1.1.2 The D_p Divergence Measure

The aforementioned divergence for probabilities $p \in (0,1)$, $q = 1-p$, and probability densities f_0 and f_1 is:

$$D_p(f_0, f_1) = \frac{1}{4pq}\left[\int \frac{(pf_0(\mathbf{x}) - qf_1(\mathbf{x}))^2}{pf_0(\mathbf{x}) + qf_1(\mathbf{x})} d\mathbf{x} - (p-q)^2\right] \tag{3}$$

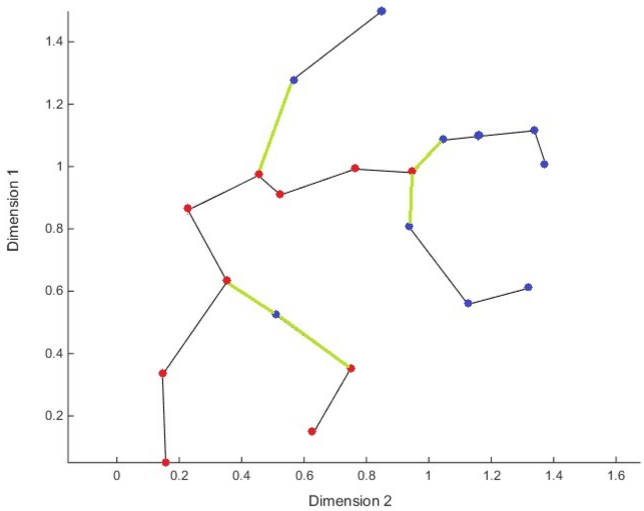
To classify D_p as a statistical distance, it must satisfy the following properties. Firstly, $0 \leq D_p$, the divergence must be non-negative. Secondly, $D_p = 0$ when $f_0(x) = f_1(x)$; the measure between identical distributions must vanish. Third, $D_p(f_0, f_1) = D_p(f_1, f_0)$, it must be symmetric. Fourth, $D_p(f_0, f_2) \leq D_p(f_0, f_1) + D_p(f_1, f_2)$, the divergence must obey the triangle inequality. D_p is shown in [25] to have the following properties: it is non-negative ($0 \leq D_p \leq 1$), satisfies the identity property, and is symmetric. However, the triangle inequality has not been proved for the measure, so therefore, we label D_p as a pseudo-distance.

The estimator for this divergence relies on finding the Friedman-Rafsky (F-R) test statistic: $\mathcal{C}(\mathbf{X}_f, \mathbf{X}_g)$ from the d-dimensional class data $\mathbf{X}_{f_0}$ and $\mathbf{X}_{f_1}$. The F-R test statistic is calculated by generating a data set containing both $\mathbf{X}_{f_0}$ and $\mathbf{X}_{f_1}$, finding the Euclidean MST for the data, and counting the number of edges of the MST that connect a point from $\mathbf{X}_{f_0}$ and $\mathbf{X}_{f_1}$. In terms of the F-R test statistic, the estimator for D_p is:

$$1 - \mathcal{C}(\mathbf{X}_{f_0}, \mathbf{X}_{f_1})\frac{N_{f_0} + N_{f_1}}{2N_{f_0}N_{f_1}} \to D_p \tag{4}$$

as $N_{f0} \to \infty$ and $N_{f_1} \to \infty$. Given that $\frac{N_{f_0}}{N_{f_0}+N_{f_1}} \to p$ and $\frac{N_{f_1}}{N_{f_0}+N_{f_1}} \to q$. Note that N_{f0} and N_{f1} are the number of samples of data from each class. Using this method, D_p is estimated from the data samples without any density estimation. The figure below graphically illustrates how the F-R test statistic is calculated.

Figure 1: Calculation of F-R Test Statistic



In Figure 1, 20 elements drawn from two uniformly distributed datasets are used to calculate $\mathcal{C}(\mathbf{X}_{f_0}, \mathbf{X}_{f_1})$. The red points are 10 elements drawn from $f_0(x) = \mathcal{U}\big([0,0]^T, [1,1]^T\big)$. The blue points are the 10 elements drawn from $f_1(x) = \mathcal{U}\big([0.5,0.5]^T, [1.5,1.5]^T\big)$. A Euclidean minimum spanning tree is created for the dataset $\mathbf{X}_{f_0} \bigcup \mathbf{X}_{f_1}$. Then, the value of the F-R statistic is equal to the number of edges of the MST that connect a data point from $\mathbf{X}_{f_0}$ to a data point from $\mathbf{X}_{f_1}$.

For Figure 1, $\mathcal{C}(\mathbf{X}_{f_0}, \mathbf{X}_{f_1}) = 5$. From the plot of the MST notice that if $\mathbf{X}_{f_0}$ and $\mathbf{X}_{f_1}$ had a greater degree of separation, there would be a fewer number of edges linking the two classes, and $\mathcal{C}(\mathbf{X}_{f_0}, \mathbf{X}_{f_1})$ would be smaller. Based on equation (4), a smaller F-R test statistic gives a larger value for the divergence estimate. However, if the two classes had more overlap, there would be a greater number of edges linking the two classes. A larger F-R test statistic would result in a smaller divergence estimate.

In [2] a modified version of this distance is proposed for implementation in binary classification tasks. As binary classification problems are considered in this work, the modified form of the distance and a modified estimator are used. Notationally, $\widetilde{D}_p$ is used to refer to the modified divergence, and D_p is used to refer to the distance itself. The same condition that $N_{f0} \to \infty$ and $N_{f_1} \to \infty$ is imposed on the estimator:

$$\widetilde{D}_p(f_0, f_1) = \int \frac{(pf_0(\mathbf{x}) - qf_1(\mathbf{x}))^2}{pf_0(\mathbf{x}) + qf_1(\mathbf{x})} d\mathbf{x} \tag{5}$$

$$1 - 2\frac{\mathcal{C}(\mathbf{X}_{f_0}, \mathbf{X}_{f_1})}{N_{f_0} + N_{f_1}} \to \widetilde{D}_p(f_0, f_1) \tag{6}$$

$\widetilde{D}_p(f_0, f_1)$ is not a distance, as it violates the identity property. If $f_0(\mathbf{x}) = f_1(\mathbf{x})$, $\widetilde{D}_p(f_0, f_1)$ is not zero in all cases. However, equation (5) is used rather than equation (3) as the Bayes error rate bounds are simpler expressed when in terms of $\widetilde{D}_p(f_0, f_1)$. Additionally, it is easy to see that in one special case, $\widetilde{D}_p = D_p$. When $p = q = 0.5$, $\widetilde{D}_p$ *does* satisfy the identity property. For all the cases we consider, $p = q = 0.5$. Therefore, $\widetilde{D}_p$ and D_p are equivalent in the context of this work.

1.2 Bayes Error Rate and Divergence Measures

A common problem in machine learning is binary classification, in which data $\mathbf{X}_i \in \mathbf{R}^{\mathbf{n}\times\mathbf{d}}$ are assigned a class label $c_i \in \{0, 1\}$. Given c_0 and c_1 correspond to data with respective probability distributions $f_0(\mathbf{x})$ and $f_1(\mathbf{x})$, prior probabilities $p \in (0, 1)$ and $q = 1 - p$, the Bayes optimal classifier assigns a class label to a test data x_i such that the posterior probability is maximized [4]. The error rate of this optimal classifier, the Bayes error rate (BER), provides an absolute lower bound on the classification error rate. Accurate estimation of the BER makes it possible to quantify the performance of a classifier with respect to this optimal lower bound, or apply improved BER bounds to feature selection algorithms [1].

Given the two conditional density functions, $f_0(\mathbf{x})$ and $f_1(\mathbf{x})$, it is possible to write the Bayes error rate in terms of the prior probabilities p and q:

$$E_{Bayes} = \int_{r_1} p f_0(\mathbf{x})\, d\mathbf{x} + \int_{r_0} q f_1(\mathbf{x})\, d\mathbf{x} \tag{7}$$

Here, r_1 and r_0 refer to the regions where the respective posterior probabilities are larger. Direct evaluation of this integral can be quite involved and impractical, and poses similar problems to that of estimation of f-divergences: it is challenging to create an exact model for the distributions $f_0(\mathbf{x})$ and $f_1(\mathbf{x})$. As an alternative to direct evaluation of the integral, it is possible to derive bounds for the Bayes error rate in terms of divergence measures [5].

The Bayes error rate can be related to the total variation distance (shown in Table 1), which itself can be written in terms of the K-L divergence [30], [31]. The Pinkser inequality [32] and related bounds are one such method to arrive at the total variation distance starting from the K-L divergence. However, as noted previously, in certain cases the K-L divergence may not be bounded, and can result in a value that tends to ∞. Vajda [33] modified the relation between the K-L divergence and the total variation distance to account for this problem.

Bounds for the classification error rate have been given in terms of the Bhattacharya distance in [33]. In [2] the Bayes error rate is given in terms $\widetilde{D}_p$:

$$\frac{1}{2} - \frac{1}{2}\sqrt{\widetilde{D}_p(f_0, f_1)} \leq E_{Bayes} \leq \frac{1}{2} - \frac{1}{2}\widetilde{D}_p(f_0, f_1) \tag{8}$$

As expected, when there is no overlap between the two distributions, $\widetilde{D}_p = 1$, and the BER is lower bounded by zero. In other words, if the two classes are highly separated, the divergence is large, and it should be possible to design a classifier that has a very low probability of error. On the other hand, if there is full overlap between the two distributions, $\widetilde{D}_p = 0$, and the BER is 0.5. In the second case, the divergence is very small, and the optimal error rate is equivalent to the error in randomly assigning class.

1.3 Bootstrap Estimation Based on Power Law

As we have just shown, the method for empirically calculating a specific D_p value for a data set of length N, and obtaining an estimate for the BER is quite straight forward, but it leaves much to be desired. Specifically, it is necessary to characterize the quality of the D_p estimate. A direct calculation of the divergence measure using all N data points yields only a single value, and does not provide any insight into the error or spread of the estimator. Indeed, in many cases knowledge of the spread of the estimate is as important as the estimate itself.

Bootstrap resampling, first introduced by Efron in [10], is a powerful tool to find the sampling distribution of a statistic. From a data set $\mathbf{X}_i$ of size N, the bootstrap method functions by repeatedly and randomly sampling, with replacement, b subsets of size $n < N$ from the original data set. Then, estimates are computed for all b generated subsets. This Monte Carlo approach gives a powerful way to analyze some measure of estimator quality (such as variance or confidence interval) from b computed estimates. However, the bootstrap with replacement fails when applied to the F-R test statistic based estimator. Because the F-R test statistic requires the generation of unique distances between data points when computing the minimum spanning tree, it is not possible to sample with replacement [2].

To satisfy the requirement, we consider another bootstrap resampling technique, the m out of N bootstrap. This technique generates i randomly sampled subsets of size $m < N$, where the subsets are generated *without replacement*. Then the quantities of interest are calculated for the i subsets. Particularly, we consider calculating the confidence interval of D_p after finding D_p for all i sample sizes. Now, we have an estimate of D_p along with a confidence interval. But, this estimate is for finite data size, and the estimator for D_p, equation (6), specifies an asymptotic condition of $N_{f0} \to \infty$ and $N_{f_1} \to \infty$. Obtaining this estimate of D_p for $N \to \infty$ is desirable in order to minimize the bias.

Hawes and Priebe [1] apply a k-Nearest Neighbors rule to find the upper and lower bound on the Bayes error rate as a function of sample size. They perform individual bootstrap estimates of the BER (which they denote as $\bar{L}_n(k)$) at many sample sizes $n_1<n_2<...<n_i<N$. Then, they apply a parametric power law curve to calculate the bootstrapped Bayes error rate estimates as a function of sample size, n. The model in question is:

$$\bar{L}_n(k) = an^b + c \tag{9}$$

with power law fit constants a, b, c, and independent variable of sample size, n. Given that this model is valid and $b < 0$, as $n \to \infty$, $\bar{L}_n(k) \to c$ with $c = \bar{L}_\infty(k)$. In [34] it is shown that $|\bar{L}_n(1) - \bar{L}_\infty(1)| \leq an^{-2}$; the absolute error of the BER estimate for a 1-dimensional data, with $k = 1$ rule, converges in the form given by equation (9).

This result was generalized in [35] for d-dimensional data. In [36] it was generalized to any choice of k, and produced the following expression for the BER:

$$\bar{L}_n(k)\ \bar{L}_\infty(k) + \sum_{j=2}^{\infty} c_j n^{-j/d} \tag{10}$$

As n increases, the term that dominates happens to be $cn^{-2/d}$. This is in agreement with the earlier described result for the $d = 1$ case. So there is strong evidence to believe that the convergence of the Bayes error rate can be given by equation (10). (Please note that for the remainder of this paper, the Bayes error rate will be referred to as E_{Bayes}, not $\bar{L}_n(k)$).

2 Methods

While Hawes and Priebe focus on obtaining asymptotic bounds of the BER, this works focuses on finding the asymptotic value for the D_p estimator. As shown in equation (8) of Section 1.2, it is possible to simply and directly relate the Bayes error rate to D_p. Therefore, the motivation behind the power law method for bounding the BER can also motivate an approach to find D_p. Though it has not been proven, it is a sensible assumption that the divergence estimates follow a similar power law for increasing sample size, and that an asymptotic estimate, $\bar{D}_p^*$, may be generated using this formulation. The following power law is defined:

$$\bar{D}_p(f_0, f_1) = an^b + c \tag{11}$$

Notice that under the sound assumption of $b < 0$, $\bar{D}_p \to c$ as $n \to \infty$. So, we have good reason to believe that from a size N, finite length data set, it is possible to obtain asymptotic estimates for the divergence. To find a measure of spread for the divergence estimator, the 95% confidence interval is calculated from the curve fitting process. Reviewing notation, D_p refers to the distance in equation (3), $\widetilde{D}_p$ is the modified version of the distance suited to binary classification given in equation (5), and is equivalent to D_p for our cases. $\bar{D}_p$ is the power law curve describing the estimator of D_p as a function of sample size from the equation above. The asymptotic value of the divergence is denoted as $\bar{D}_p^*$.

2.1 Algorithm for $\bar{D}_p^*$ Calculation

Input: Data $\mathbf{X}_0, \mathbf{X}_1 \in \mathbf{R^{n \times d}}$ of length N, dimensionality $\mathbf{d}$
m: number of Monte Carlo iterations
i: number of bootstrap subsample sizes $\mathbf{n}_i \in \{n_1, n_2, ..., n_i < N\}$
$\mathbf{X}_S = \mathbf{X}_0 \bigcup \mathbf{X}_1$
Result: Asymptotic estimate of D_p : $\bar{D}_p^*$
Power law curve: $\mathcal{P}(\bar{\mathbf{D}}_{p_i}, \mathbf{n}_i) = \bar{D}_p(f_0, f_1) = an^b + c$

Define: $\bar{\mathbf{D}}_{p_i} = \{\bar{D}_{p_1}, \bar{D}_{p_2}, ..., \bar{D}_{p_i}\}$, mean Monte Carlo estimate for each sample size n_i

for $i \in n_1, n_2, ..., n_i$ **do**
Define empty array $\mathbf{D}_p = \{D_{p_1}, D_{p_2}, ..., D_{p_m}\}$, containing the m Monte Carlo estimates

for $k \in 1...m$ **do**
Randomly sample a length n_i subset: $\mathbf{S} = \{x_1, ..., x_{n_i}\}$ from $\mathbf{X}_S$, without replacement
// Ensure $N_{S,0} = N_{S,1}$, number of data samples from each class must be equal

// Compute k^{th} Monte Carlo estimate
$D_{p_k} = 1 - 2\frac{\mathcal{C}(\mathbf{S}_0, \mathbf{S}_1)}{N_{S,0} + N_{S,1}}$
end
// Bootstrapped estimate $\bar{D}_{p_i}$ is the average of the D_{p_k}
$\bar{D}_{p_i} = \frac{1}{m} \sum_{k=1}^{m} D_{p_k}$
end

// Apply the power law
$\{a, b, c\} = \mathcal{P}(\bar{\mathbf{D}}_{p_i}, \mathbf{n}_i)$
$\bar{D}_p^* = c$

Algorithm 1: Algorithm for finding asymptotic divergence value $\bar{D}_p^*$

The algorithm for finding the $\bar{D}_p^*$ value for a two class data set follows from the overview of bootstrap sampling in 1.3. After deciding the target two class dataset, m, the number of Monte Carlo iterations, must be defined. Then, choose i and $\mathbf{n}_i$, the number of bootstrap subsamples and the bootstrap subsample sizes. Begin with the outer loop, and iterate through the number bootstrap subsample sizes, i. Create a randomly sampled subset $\mathbf{S}$ of length n_i from the data $\mathbf{X}_S$ containing an equal number of elements from each class, and compute the divergence estimate for the subset $\mathbf{S}$. Repeat the subset creation and divergence estimation m times (this is the inner loop). Upon returning to the outer loop, find the mean of the m D_{p_k} values. Once the mean value of m estimates for all i bootstrap subsample sizes has been found, apply the power law fit, $\mathcal{P}$, to the mean values and subsample sizes. The asymptotic value of the divergence estimator $\bar{D}_p^*$ is equal to c.

We note several restrictions on input parameters. Define maximum value of subsample size as n_{max}. This value must be less than N. Also, N choose n_{max} must be greater than m. This is a requirement for sensible Monte Carlo iterations: there must be at least m unique subsets of size n_{max}. From the lower extreme of subsample size, n_1 must be greater than the number of dimensions of the data set.

3 Results

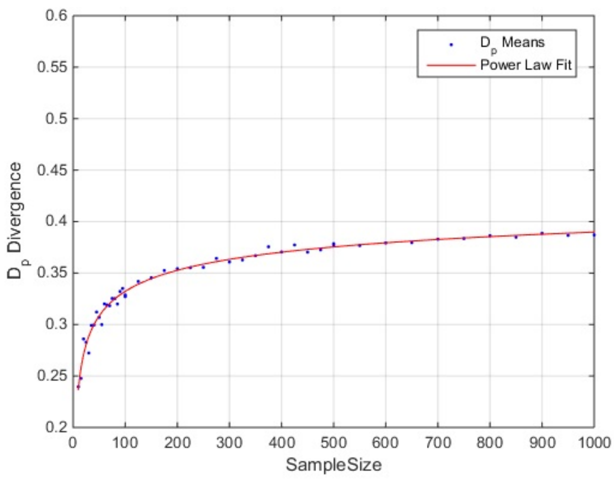
3.1 Uniform Dataset

To test the operation of the estimation algorithm, a data set with a known divergence is constructed in order to ensure that the computed value of $\bar{D}_p^*$ matches with the known divergence. For this purpose, the uniform distribution shown in Table 2 is defined. The data set contains 8 dimensions, all of which have variance $\sigma^2 = \frac{1}{12}$, and are uniformly distributed along $[-0.5, 0.5]$, with the exception of one dimension from c_1. That dimension has an offset mean of $\mu_1 = \frac{1}{2}$ rather than $\mu_1 = 0$. It is easy to see that a direct application of equation (3) or (5) results in a divergence value of $D_p = 0.5$. Refer to the Appendix for this computation.

Table 2: Uniform Dataset for Analysis of D_p

c_0								
μ_0	0	0	0	0	0	0	0	0
σ_0^2	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$
c_1								
μ_1	$\frac{1}{2}$	0	0	0	0	0	0	0
σ_1^2	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$

Figure 2: Asymptotic Convergence of D_p for 8-Dimensional Uniform Data Set, m = 200 trials



To find $\bar{D}_p^*$, a 10000 point dataset containing an equal number of instances from both classes c_0 and c_1 was created. With respect to Algorithm 1, the parameters of the simulation were: $N = 10000$, $m = 200$ Monte Carlo iterations, $i = 50$ bootstrap subsample sizes, and $n_{max} = n_{50} = 1000$ as the maximum bootstrap sample size. The results of the simulation are shown in Figure 1. The plot shows computed estimates of D_p as a function of sample size and displays the resulting power law fit. Each blue point on the figure is a D_p mean - the mean of 200 Monte Carlo trials at each bootstrap sample size n_i.

The power law found for D_p for this uniform dataset is:

$$\bar{D}_p = -0.39n^{-0.22} + 0.4775 \tag{12}$$

The asymptotic estimate $\bar{D}_p^* = 0.4775$ is in approximate agreement with the analytically calculated value for the dataset, $\mathbf{D}_p = 0.5$. To understand the true capability of the power law based, asymptotic estimation method consider Table 3.

Table 3: Estimated D_p for Uniform Data Set for $n_{max} = 1000$

Value	Result (95% Confidence Interval)
$\mathbf{D}_p$ (true value)	0.5
D_p (no Bootstrap)	0.3370
D_{p_mean}	0.3870 (0.3422, 0.4288)
$\bar{D}_p^*$	**0.4775** (0.4378, 0.5173)

When a direct computation of the divergence measure is performed for 1000 data points an estimate of $D_p = 0.337$ is obtained. This is problematic for two reasons. As explained earlier, there is no information about the distribution of the estimate. Additionally, the calculated value $D_p = 0.337$, is far from the true value of $D_p = 0.5$. The result is of little use for any application.

$\bar{D}_{p\_mean}$ is the average of $m = 200$ Monte Carlo estimates for a subsample size of 1000. Because the distribution of the estimates are approximately Gaussian, a crude way to characterize the 95% confidence interval of the estimator is to consider values within 2σ of the mean. But, the resulting confidence interval and value $D_{p\_mean} = 0.3870$ are only marginally better than the value found without bootstrapping iterations, and still have large errors.

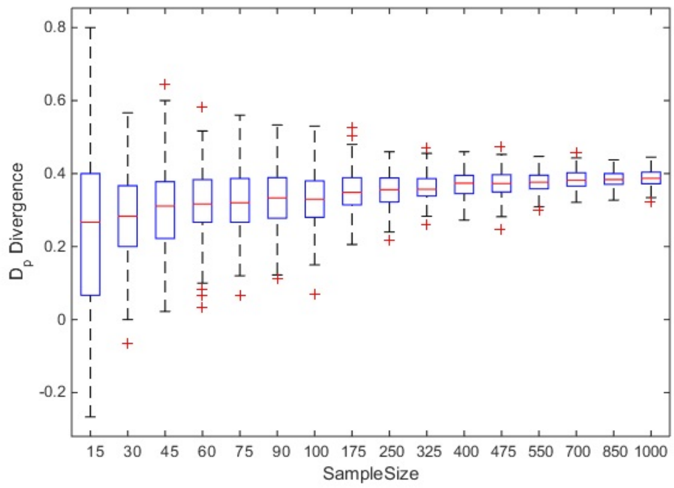
If we then consider the asymptotic power law estimate $\bar{D}_p^* = 0.4775$ with confidence interval $(0.4378, 0.5173)$, we see that the value of $\bar{D}_p^* = 0.4775$ is fairly close to the true value of $\mathbf{D}_p = 0.5$. This result is far more favorable than the previous results. Additionally, the confidence interval found via the power law fit process includes the true value. Through this example, we have confirmed our assumption that the power law can be applied to find the asymptotic divergence estimate.

Proper Selection of $\mathbf{n}_i$

While selecting the set of subsample sizes $\mathbf{n}_i \in \{n_1, n_2, ..., n_i < N\}$, it is vital that a significant portion of the i subsample sizes are concentrated within the rapidly rising portion of the power law curve. In Figure 1, notice that for a sample size of up to $n = 200$, the estimates of divergence change rapidly for increasing sample size. But, for $n > 200$, the convergence of the estimates slows - the divergence estimates change slowly for increasing sample size greater than 200. In this case the n_i are chosen so that n_1 to n_{20} are spaced evenly on the interval $[8, 100]$ (n_1 should not be smaller than the number of dimensions). Then, n_{21} to n_{40} are evenly spaced for $[100, 500]$. Finally, n_{41} to n_{50} are evenly spaced between $[500, 1000]$.

Although the exact choice of $\mathbf{n}_i$ may differ between each use case, a useful heuristic to ensure a good power law fit is described. Take the maximum bootstrap subsample size to be $n_{max} < N$. In this case, $n_{max} = 1000$. Choose approximately $\frac{1}{3}$ of the n_i subsamples on the interval $(0, 0.1n_{max})$, choose $\frac{1}{3}$ of the subsamples between $(0.1n_{max}, 0.5n_{max})$, and choose the final $\frac{1}{3}$ in the interval $(0.5n_{max}, n_{max})$. If there are fewer number of subsamples n_i that are small relative to n_{max}, or if n_i are evenly spaced along $(0, n_{max})$, the goodness of fit for the power law is likely to be compromised. If n_i must be evenly spaced, we may increase the number of subsamples, i, and decrease the space between each subsample size to try and preserve a good curve fit.

Figure 3: Distribution of D_p Values for 8-Dimensional Uniform Data Set, m = 200 trials



An additional benefit of increasing the subsample size, is that the spread of estimator decreases. The same data used to create Figure 1 are shown in Figure 2 to emphasize the decrease in estimator's spread. Recognize that the x-axis is not linearly scaled, and that the y-axis does not have the same scale as Figure 1. For every D_p point plotted in Figure 1 (every blue point), $m = 200$ Monte Carlo estimates have been averaged. In Figure 2, box plots of the 200 Monte Carlo iterations are shown for select values of subsample size. Although every single average D_p value plotted in Figure 1 has a corresponding box plot, only a select number of box plots are shown due to limited space, and to avoid cluttering Figure 2. Here, the estimator's bias for small sample sizes is clearly visible in the $n = 15$ case, as negative values are produced. But, as sample size increases, there is a dramatic reduction in the interquartile range.

3.2 Gaussian Dataset

Table 4: Gaussian Dataset for Analysis of D_p

c_0								
μ_0	0	0	0	0	0	0	0	0
σ_0	1	1	1	1	1	1	1	1
c_1								
μ_1	2.56	0	0	0	0	0	0	0
σ_1	1	1	1	1	1	1	1	1

We wish to show that this estimation method is valid for many types of distributions. Therefore, we now consider the 8-dimensional Gaussian dataset given in Table 4 [37]. All dimensions of the data are zero mean and unit variance except for the first dimension of class 1. The mean of one of the dimensions of c_1 is shifted to $\mu_1 = 2.56$. It is not possible to analytically calculate D_p for a Gaussian dataset. But, the Bayes error rate for this data set is known (BER=10%). So, $\bar{D}_p^*$ can be validated by calculating the bounds on the BER from $\bar{D}_p^*$, and comparing to the known BER value.

The same conditions as Section 3.1 are applied. A 10000 instance dataset is created containing an equal number of points from both classes. The number of Monte Carlo iterations $m = 200$, and bootstrap subsample sizes $\mathbf{n}_i$ are selected in the same manner with $n_{max} = 1000$. The only difference in this case is that a Gaussian dataset is analyzed rather than a Uniform dataset, and an additional step of computing the BER is performed. The resulting power law curve for this dataset is:

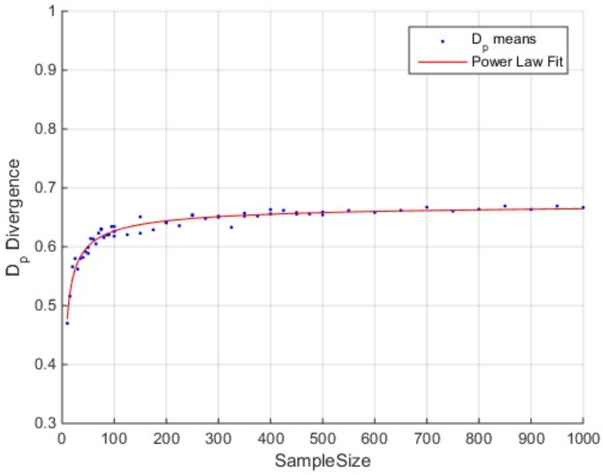
$$\bar{D}_p = -0.79n^{-0.59} + 0.6773 \tag{13}$$

with asymptotic divergence estimate and confidence interval: $\bar{D}_p^* = 0.6773$ (0.6687, 0.686). Applying equation (8), Table 5 contains resultant bounds on the BER. The true value of the Bayes error rate is within the upper and lower bounds found via the value $\bar{D}_p^*$. So, $\bar{D}_p^*$ has been successfully estimated for the Gaussian case. Refer to Figure 3 for a plot of equation (13).

Table 5: Estimated Bayes Error Rate for Gaussian Data Set for $n_{max} = 1000$ [4]

Quantity	Bayes Error
True Value	10 %
Estimated Lower Bound	$8.85\% \pm 0.26\%$
Estimated Upper Bound	$16.13\% \pm 0.43\%$

Figure 4: Asymptotic Convergence of D_p for Gaussian Data Set, m = 200 trials



3.3 Banknote Dataset

The first real world example considered is the Banknote Authentication Data Set taken from the University of California, Irvine Machine Learning Repository [7]. The dataset is 4-dimensional, and has $N = 1372$ instances. The features of the dataset are extracted from images of genuine and forged banknotes, and the classification task is to label a data vector as either forged or genuine. The dataset consists of a relatively small number of dimensions and highly separated data, so the convergence is rapid, even for relatively small sample size.

The following parameters for Algorithm 1 are set: $m = 50$, $i = 50$, $n_{max} = 600$, and most subsamples sizes n_i are less than $0.5n_{max}$. For a sensitive task such as authenticating banknotes, it should not be surprising to see an asymptotic value for D_p that is almost equal to 1:

$$\bar{D}_p = -3.18n^{-0.98} + 1.001 \tag{14}$$

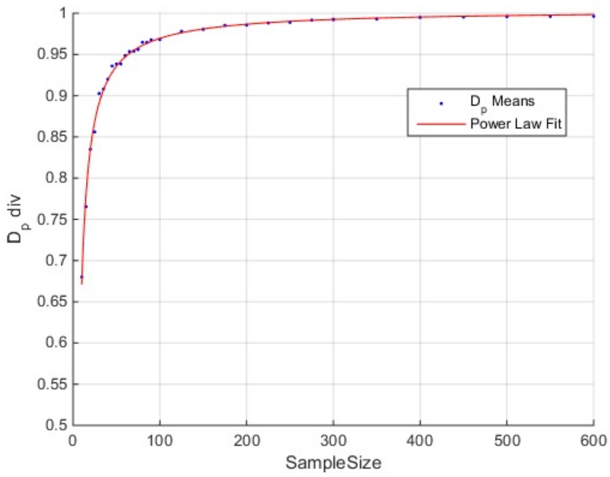
This curve is plotted in Figure 4, along with the means of the $m = 50$ Monte Carlo trials. The asymptotic value of the divergence estimate and its 95% confidence interval is $\bar{D}_p^* = 1.000(0.997, 1.005)$.

Table 6: Estimated Bayes Error Rate For Banknote Data Set

Quantity	Bayes Error
Estimated Lower Bound	$-0.02\% \pm 0.09\%$
Estimated Upper Bound	$-0.05\% \pm 0.20\%$

If equation (8) is applied, the lower and upper bound of the BER are both negative: (-0.02%, -0.05 %). Because a negative error rate is nonsensical, for this dataset the Bayes error rate is taken as 0%. This means that an optimal classifier for this dataset could hope to make no errors at all in sorting banknotes as forged or genuine. This is certainly good news!

Figure 5: Convergence of D_p for Banknote Authentication Data Set, m = 50 trials



3.4 Pima Indian Dataset

The second real world dataset analyzed is the Pima Indian Dataset, also sourced from the UCI Machine learning repository [38]. The dataset has 8-dimensions containing clinical information such as age, blood pressure, BMI, and plasma glucose concentration about female patients of Pima Indian heritage who are age 21 or older. Class 1 corresponds to patients with diabetes, and class 0 contains patients without diabetes. Due to the relatively low number of instances in the dataset, it is of particular interest to find an asymptotic value of the divergence estimator.

Of the $N = 768$ instances, 500 belong to class 0, and 268 instances are from class 1. In the discussion of equations (5) and (6) it was noted that in order for the condition $\widetilde{D}_p = D_p$ to hold, $p = q = 0.5$. Therefore the maximum subsample size is limited to $n_{max} < 2 * 268$ because calculation of the divergence estimate requires an equal number of data samples from each class to ensure $p = q = 0.5$. For this dataset, an analysis of the effect of varying m, and n_{max} is performed. The increment between each subsample size n_i is 2, so the number of bootstrap sample sizes i, is large.

In Table 7, the results of varying n_{max} and m are shown. Each row of the table corresponds to applying Algorithm 1 with the specified n_{max} and m. As expected, when the number of Monte Carlo iterations is increased for a fixed n_{max}, the 95% confidence interval for the asymptotic estimate tightens. Remarkably, the performance of the algorithm for small values of maximum sample size is comparable to the results of larger sample sizes.

When $n_{max} = 100$ and $m = 5000$, the lower bound on the BER is 22.13 $\pm$ 0.67 %. All other cases of $m = 5000$ produce results for the BER lower bound that are within this confidence interval. In fact, there are only a few cases in Table 7 where the lower bound of the BER is outside this confidence interval. Even with the seemingly restrictive maximum sample size of $n_{max} = 100$, estimates for the BER are accurate. This speaks to the strength of the power law based estimation method.

To understand the effect of changing m, refer to Figures 5-7 and the confidence intervals in Table 7. Figures 5-7 plot the power law curves for the results given in the last three rows of Table 7. In every case, a smaller value for m results in a larger confidence interval. This can be seen visually in the spread of the means of the m Monte Carlo Iterations about the fitted curve. The $D_{p_{means}}$ have the greatest spread in Figure 5, where m is the smallest. In Figure 6, the larger value of m results in $D_{p_{means}}$ that are closer to the fitted curve. When a large value of 5000 is chosen for m, the result is plotted in Figure 7. There is an almost exact fit between the power law model and the Monte Carlo means. So, as the number of Monte Carlo iterations are increased, the variability from the random sampling process is reduced, and the computed estimates lie almost exactly on the predicted curve.

Table 7: D_p and Bayes Error Rate for the Pima Indian Data Set for Increasing Sample Size and Monte Carlo Iterations

Sample Size n_{max}	Monte Carlo Iterations m	$\bar{D}_p^*$ (95% CI)	Bayes Error Rate (%), ($\pm$ 95% CI) Lower Bound	Bayes Error Rate (%), ($\pm$ 95% CI) Upper Bound
100	50	0.2725 (0.245, 0.3)	23.90 ± 1.32	36.38 ± 1.38
100	200	0.2958 (0.265, 0.3267)	22.81 ± 1.42	35.21 ± 1.54
100	5000	0.3107 (0.2959, 0.3254)	22.13 ± 0.67	34.47 ± 0.75
200	50	0.2946 (0.2732, 0.3161)	22.86 ± 0.99	35.27 ± 1.07
200	200	0.3029 (0.288, 0.3178)	22.48 ± 0.68	34.86 ± 0.74
200	5000	0.3162 (0.3114, 0.3209)	21.88 ± 0.21	34.19 ± 0.24
300	50	0.3118 (0.2827, 0.3409)	22.08 ± 1.31	34.41 ± 1.46
300	200	0.3073 (0.2926, 0.3219)	22.28 ± 0.66	34.63 ± 0.74
300	5000	0.3041 (0.3006, 0.3075)	22.43 ± 0.16	34.79 ± 0.18
500	50	0.2886 (0.2855, 0.2917)	23.14 ± 0.14	35.57 ± 0.15
500	200	0.2895 (0.2871, 0.2918)	23.10 ± 0.11	35.53 ± 0.12
500	5000	0.2963 (0.2939, 0.2987)	22.78 ± 0.11	35.19 ± 0.12

In Section 3.1 the results of various methods of estimating D_p were compared with the asymptotic method. Rather than compare the results of various D_p estimation methods for the Pima Indian dataset, the Bayes error rates resulting from these estimation methods are compared. In Table 8, the resulting Bayes error rate is calculated for three estimation methods. In the first method (no bootstrap), a single computation of D_p is performed for 500 points drawn from the dataset. Though the computed BER from this method is comparable to the BER bounds calculated with the asymptotic estimate, there is know knowledge of the uncertainty in this result.

The Bayes error calculated from $D_{p_{means}}$, the mean of $m = 5000$ Monte Carlo iterations, is very similar to the non-bootstrapped estimate of the BER. Recall that the confidence interval for $D_{p_{means}}$ is given by recognizing that the sampling distribution of the Monte Carlo estimates are approximately gaussian. Therefore, the 95 % CI for $D_{p_{means}}$ is created by including values within 2σ.

Table 8: Bootstrap Estimated Bayes Error Rates for Pima Indians Data Set, $n_{max} = 500$, $m = 5000$ [4]

Estimator Used	Bayes Error Rate (%), (± 95% CI) Lower Bound	Bayes Error Rate (%), (± 95% CI) Upper Bound
D_p (no Bootstrap)	23.32 (No CI)	35.72 (No CI)
$D_{p_{means}}$	23.26 ± 2.73	35.69 ± 3.08
$\bar{D}_p^*$	$\mathbf{22.78 \pm 0.11}$	35.19 ± 0.12

Table 9: Bayes Error Rates in Literature for Pima Indians Data Set [4]

Algorithm	Bayes Error Rate (%)
Discrim	22.50
Quadisc	26.20
Logdisc	22.30
SMART	23.20
ALLOC80	30.10
K-NN	32.40
CASTLE	25.80
CART	25.50
IndCART	27.10
NewID	28.90
AC2	27.60
Baytree	27.10
NaiveBay	26.20
CN2	28.90
C4.5	27.00
Itrule	24.50
Cal5	25.00
Kohonen	27.30
DIPOL92	22.40
Backprob	24.80
RBF	24.30
LVQ	27.20

Figure 6: Asymptotic Convergence for Pima Indian Data Set, m = 50 trials

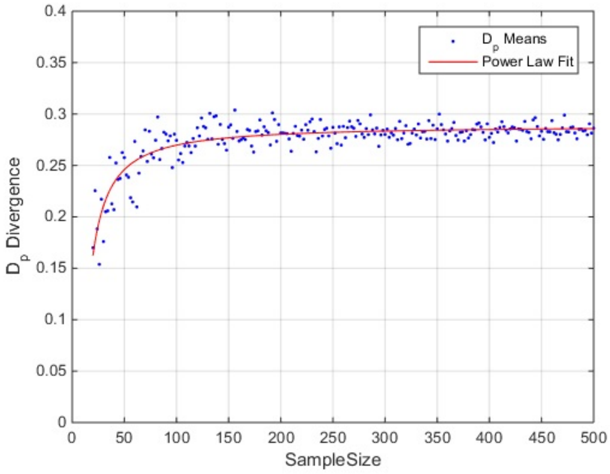


Figure 7: Asymptotic Convergence for Pima Indian Data Set, m = 200 trials

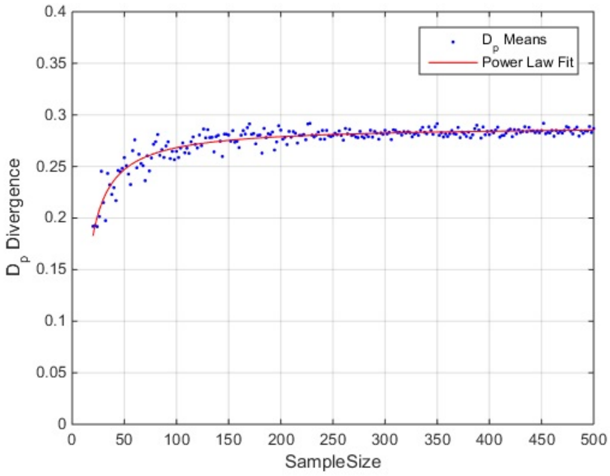


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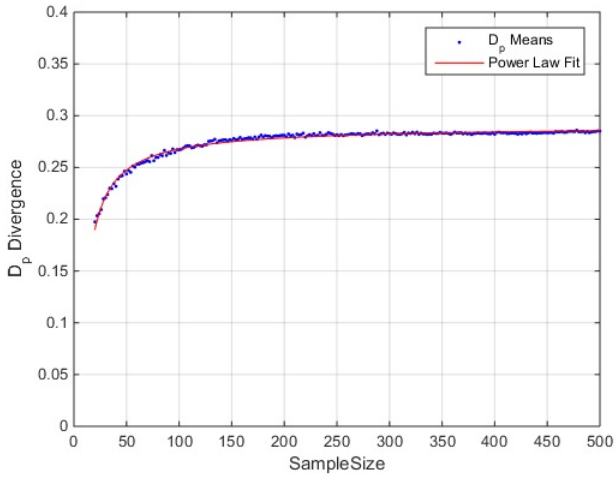
Figure 8: Asymptotic Convergence for Pima Indian Data Set, m = 5000 trials



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