Bootstrap Estimation of a Non-Parametric Information Divergence Measure

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Abstract

This work details the bootstrap estimation of a non-parametric information divergence measure, the D_p divergence measure, in the context of a binary classification problem. To address the limitation posed by a finite size data set, a bootstrap approach - suggested by Hawes and Priebe - is used to calculate an asymptotic estimate of the divergence measure. Bootstrap estimates of D_p are found for increasing values of sample data size, and a power law fit is used to find the asymptotic convergence value of the divergence measure as a function of sample size. The fit is also used to generate a confidence interval for the estimate which allows us to characterize the quality of the estimator. The results obtained for the divergence measure are then compared to several other resampling methods. Utilizing 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 the power law estimation approach for D_p.

1 Introduction

Information divergence measures have a wide variety of applications in machine learning, pattern recognition, statistics, and big data analysis [8]. Due to their wide range of applications, there has been particular interest in estimation of these information theoretic quantities [].

Equally important to estimating

The Binary Classification Problem

A common problem in machine learning is the binary classification problem, in which data $x_i \in \mathbf{R^n}$ is assigned a class label $c_i \in \{0, 1\}$ according to a classification rule, where class labels c_0 and c_1 correspond to respective probability distributions $f_0(\mathbf{x})$ and $f_1(\mathbf{x})$. The Bayesian classifier assigns class labels to x_i such that the posterior probability is maximized. The error rate of this classifier, the Bayes error rate, provides an absolute lower bound on the classification error rate. Estimating the best achievable classification error rate makes it possible to quantify the usefulness of a feature set or the performance of a classifier [1].

Given the two conditional distributions, $f_0(\mathbf{x})$ and $f_1(\mathbf{x})$, it is possible to write the Bayes error rate in terms of the prior probabilities p_0 and p_1 as given in [2]:

$$E_{Bayes} = \int_{r_1} p_0 f_0(\mathbf{x})\, dx + \int_{r_0} p_1 f_1(\mathbf{x})\, dx \tag{1}$$

Here, r_1 and r_0 refer to the region where the corresponding posterior probability is larger[5].

Direct evaluation of this integral can be quite involved and impractical, as it is challenging to create an exact model for the posterior distributions $f_0(\mathbf{x})$ and $f_1(\mathbf{x})$. As an alternative to direct evaluation, it is possible to derive bounds for the Bayes error rate.

We arrive at an estimate of the Bayes error rate by using expressions that give bounds on the classification error in terms of information divergence measures. However, common methods of estimating the Bayes error rate via divergence measure still require information about the conditional distributions corresponding to both class labels. Therefore the non-parametric divergence measure given in [3] will be used in conjunction with the Bayes error estimates derived for this divergence measure in [2] to conduct the analysis.

The work is organized as follows: the remainder of Section 1 is devoted to previous work, Section 2 provides a description of the divergence measure used, and its relation to the Bayes error rate, and Section 3 introduces the bootstrap sampling method, and the power law used to estimate D_p. In Section 4 we will apply the method to several generated datasets and real world datasets to show that the power law method can successfully be applied to several distributions. In 4.1 we will consider the generated example datasets, and in 4.2 we will perform our analysis on the Pima Indians dataset and the Banknote dataset found in the University of California, Irvine machine learning repository [6].

2

Previous Work

2 The D_p Divergence Measure

3 Bootstrap Sampling

As we have just shown, the method for empirically calculating a specific D_p value for a dataset of length N is quite straight forward, but it leaves much to be desired. Specifically, it is desirable 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 statistic.

Because bounds on the Bayes Error Rate can be calculated directly from D_p, Resampling techniques such as the jackknife[9], and the bootstrap[10] can be applied to find the statistical distribution of the estimated quantity in question.

Bootstrap resampling, first introduced in , is a powerful method to find the sampling distribution of an estimator. Given a In order to characterize the While the D_p value provides an insight into the separation of the data Given a dataset of size N and dimensionality D, we have established how to calculate the D_p value. How

4 Methods

Data: this text
Result: how to write algorithm with LaTeX2e
initialization;
while *not at end of this document* **do**
    read current;
    if *understand* **then**
        go to next section;
        current section becomes this one;
    else
        go back to the beginning of current section;
    end
end

Algorithm 1: How to write algorithms

5 Results

Uniform Dataset

Table 1: Uniform Dataset for Bootstrap Analysis of D_p

D_0								
μ_0	0	0	0	0	0	0	0	0
σ_0	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$
D_1								
μ_1	$\frac{1}{2}$	0	0	0	0	0	0	0
σ_1	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{1}{12}$

Gaussian Dataset

Figure 1: Asymptotic Convergence of D_p for 8-Dimensional Uniform Data Set, N = 200 trials

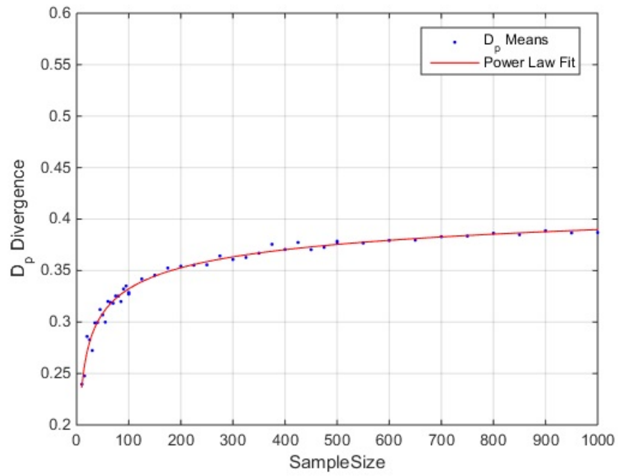
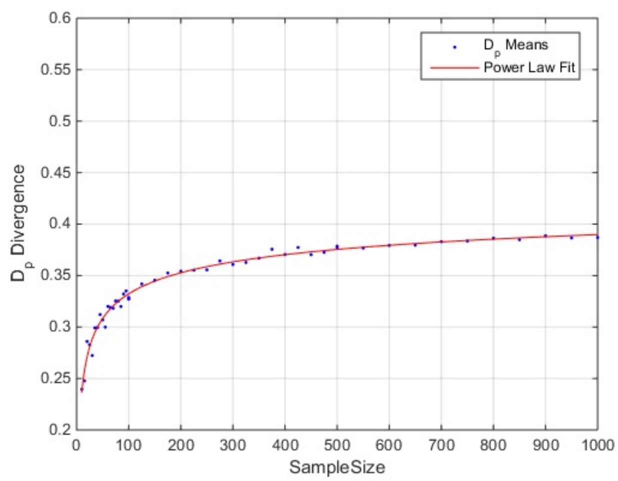


Figure 2: Distribution of D_p Values for 8-Dimensional Uniform Data Set, N = 200 trials



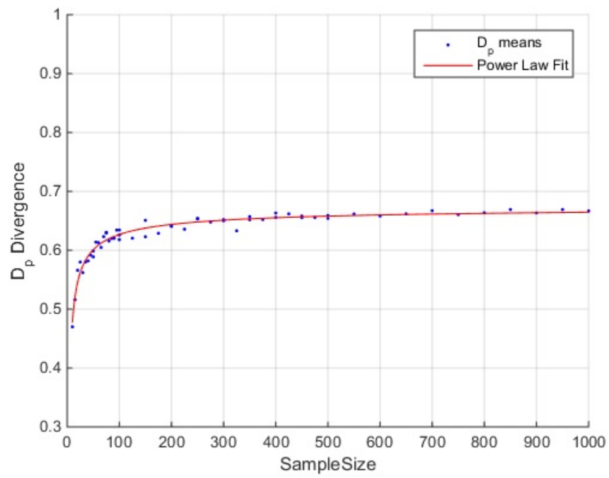
Banknote Dataset

The first real world example we consider is the Banknote Authentication Data Set taken from the University of California, Irvine Machine Learning Repository [7]. The 4-dimensional dataset contains data extracted from images of banknotes. The data set consists of a relatively small number of dimensions, and highly

Table 2: Gaussian Dataset for Bootstrap Analysis of D_p

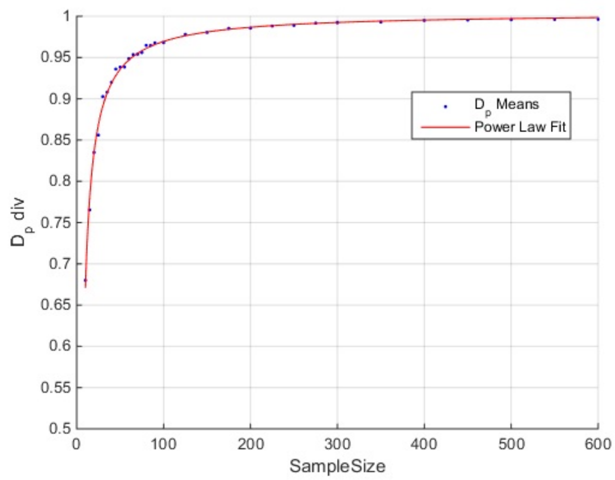
D_0								
μ_0	0	0	0	0	0	0	0	0
σ_0	1	1	1	1	1	1	1	1
D_1								
μ_1	0	0	0	0	0	0	0	0
σ_1	2.56	1	1	1	1	1	1	1

Figure 3: Asymptotic Convergence of D_p for Gaussian Data Set, N = 50 trials



separated data, so the convergence is . We note that for a sensitive task such as authenticating banknotes, it should not be surprising to see an asymptotic value for D_p that is close to 1.

Figure 4: Convergence of D_p for Banknote Authentication Data Set, N = 50 trials



Pima Indians Dataset

Figure 5: Asymptotic Convergence for Pima Indian Data Set, N = 50 trials

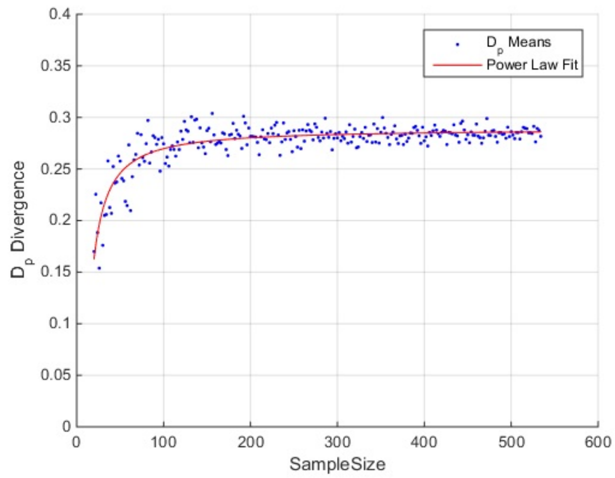


Figure 6: Asymptotic Convergence for Pima Indian Data Set, N = 200 trials

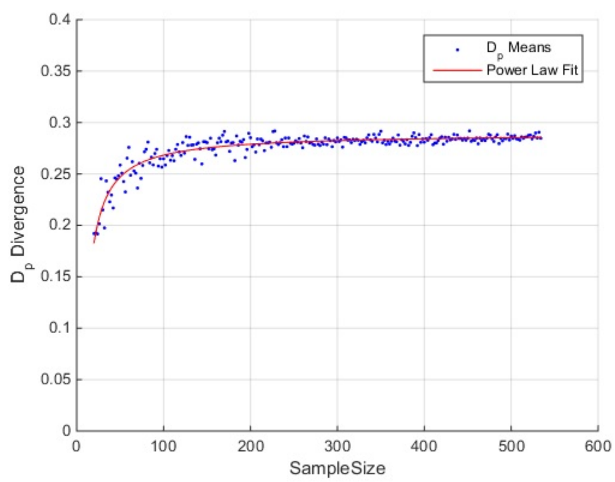
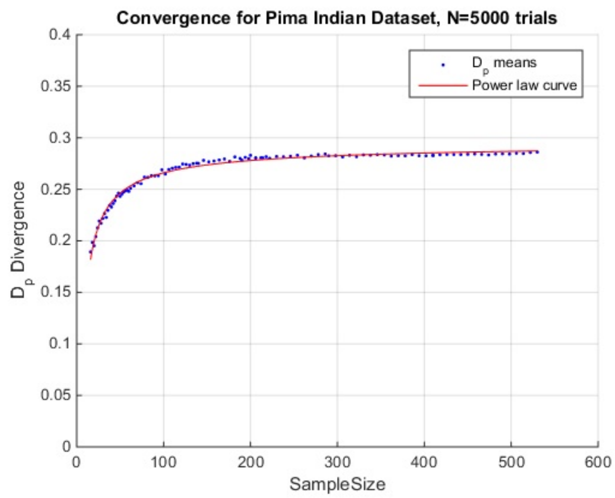


Figure 7: Asymptotic Convergence for Pima Indian Data Set, N = 5000 trials



References

[!h] [1] Hawes, Chad M., and Carey E. Priebe. "A Bootstrap Interval Estimator for Bayes' Classification Error." 2012 IEEE Statistical Signal Processing Workshop, 2012

[2] V. Berisha, A. Wisler, A.O. Hero, and A. Spanias, "Empirically Estimable Classification Bounds Based on a Nonparametric Divergence Measure" IEEE Transactions on Signal Processing, vol. 64, no. 3, pp.580-591, Feb. 2016.

[3] A. O. Hero, B. Ma, O. Michel, and J. Gorman, Alpha-divergence for classification, indexing and retrieval, Communication and Signal Processing Laboratory, Technical Report CSPL-328, U. Mich, 2001

[4] K. Tumer, K. (1996) "Estimating the Bayes error rate through classifier combining" in Proceedings of the 13th International Conference on Pattern Recognition, Volume 2, 695699

Contains the pima indian dataset BERs in table format

[5] Tumer, Kagan, and Joydeep Ghosh. "Bayes Error Rate Estimation Using Classifier Ensembles." International Journal of Smart Engineering System Design 5.2 (2003): 95-109.

[6] Lichman, M. (2013). UCI Machine Learning Repository [http://archive.ics.uci.edu/ml]. Irvine, CA: University of California, School of Information and Computer Science.

[7] V. Lohweg, Banknote Authentication Data Set, 2012. [Online]. Available: https://archive.ics.uci.edu/ml/datasets/banknote+authentication.

Table 3: 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

Table 4: Bootstrap Estimated Bayes Error Rates for Pima Indians Data Set [4]

Algorithm	Bayes Error Rate (%)
D_p (no Bootstrap)	29.32 ± 6.22 *
Efron Bootstrap	14.87 ± 2.465 **
$m < n$ Bootstrap, $m = 200$	23.13 ± 4.13
D_p **Asymptotic Power Law**	$\mathbf{23.95 \pm 0.11}$

[8] K. Pranesh, and L. Hunter. "On an Information Divergence Measure and Information Inequalities." (n.d.): n. pag. University of Northern British Columbia.

[9] Tukey, J.W. 1958. Bias and confidence in not-quite large samples. Annals of Mathematical Statistics 29: 614
Efron, B. "Bootstrap Methods: Another Look at the Jackknife." Annals of Statistics 7.1 (1979)

Table 5: D_p and Bayes Error Rate for the Pima Indian Data Set for Increasing Sample Size, and Increasing Monte Carlo Iterations

Sample Size	Monte Carlo Iterations	D_p Asymptotic Value (95% Confidence Interval)	Bayes Error Rate (%), (95% CI)
100	50	0.2725 (0.245, 0.3)	23.90 ± 1.32
100	200	0.2958 (0.265, 0.3267)	22.81 ± 1.42
100	5000	0.3107 (0.2959, 0.3254)	22.13 ± 0.67
200	50	0.2946 (0.2732, 0.3161)	22.86 ± 0.99
200	200	0.3029 (0.288, 0.3178)	22.48 ± 0.68
200	5000	0.3162 (0.3114, 0.3209)	21.88 ± 0.21
300	50	0.3118 (0.2827, 0.3409)	22.08 ± 1.31
300	200	0.3073 (0.2926, 0.3219)	22.28 ± 0.66
300	5000	0.3041 (0.3006, 0.3075)	22.43 ± 0.16