IDIAP RESEARCH REPORT

SURPRISING OUTCOME WHILE BENCHMARKING STATISTICAL TESTS

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IDIAP–RR 05-38

AUGUST 23, 2005

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Surprising Outcome While Benchmarking Statistical Tests

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Abstract. Although non-parametric tests have already been proposed for that purpose, statistical significance tests for non-standard measures (different from the classification error) are less often used in the literature. This paper is an attempt at empirically verifying how these tests compare with more classical tests, on various conditions. More precisely, using a very large dataset to estimate the whole "population", we analyzed the behavior of several statistical test, varying the class unbalance, the compared models, the performance measure, and the sample size. A surprising conclusion is that paired tests such as McNemar badly fail when comparing models which are similar (such as SVMs with different kernels). On the other hand, non-parametric tests were relatively robust to class unbalance and the *closeness* of the models.

Contents

1 Introduction

Statistical tests are often used in machine learning in order to assess the performance of a new learning algorithm or model over a set of benchmark datasets, with respect to the state-of-the-art solutions. Several researchers (see for instance [4] and [8]) have proposed statistical tests suited for 2-class classification tasks where the performance is measured in terms of the classification error (ratio of the number of errors and the number of examples), which enables the use of assumptions based on the fact that the error can be seen as a sum of random variables over the evaluation examples. On the other hand, various research domains prefer to measure the performance of their models using different indicators, such as the F_1 measure, used in information retrieval [10], described in Section 2.1. Most classical statistical tests cannot cope directly with such measure as the usual necessary assumptions are no longer correct, and non-parametric bootstrap-based methods are then used [5].

Since several papers already use these non-parametric tests [2, 1], we were interested in verifying empirically how reliable they were. For this purpose, we used a very large text categorization database (the extended Reuters dataset [9]), composed of more than 800000 examples, and concerning more than 100 categories (each document was labelled with one or more of these categories). We purposely set aside the largest part of the dataset and considered it as the whole population, while a much smaller part of it was used as a training set for the models. Using the large set aside dataset part, we *tested* the statistical test in the same spirit as was done in [4], by sampling evaluation sets over which we observed the performance of the models and the behavior of the significance test.

Following the taxonomy of questions of interest defined by Dietterich in [4], we can differentiate between statistical tests that analyze learning algorithms and statistical tests that analyze classifiers. In the first case, one intends to be robust to possible variations of the train and evaluation sets, while in the latter, one intends to only be robust to variations of the evaluation set. While the methods discussed in this paper can be applied alternatively to both approaches, we concentrate here on the second one, as it is more tractable (for the empirical section) while still corresponding to real life situations where the training set is fixed and one wants to compare two solutions (such as during a competition).

In order to conduct a thorough analysis, we tried to vary the evaluation set size, the class unbalance, the error measure, the statistical test itself (with its associated assumptions), and even the *closeness* of the compared learning algorithms. This paper, and more precisely Section 3, is a detailed account of this analysis. As it will be seen empirically, the *closeness* of the compared learning algorithms seems to be a decisive factor on the resulting quality of the statistical tests: comparing an MLP and an SVM yields much more reliable statistical tests than comparing two SVMs with a different kernel. To the best of our knowledge, this has never been considered in the literature of statistical tests for machine learning.

2 A Statistical Significance Test for the Difference of F_1

Let us first remind the basic classification framework in which statistical significance tests are used in machine learning. We consider comparing two models A and B on a two-class classification task where the goal is to classify input examples x_i into the corresponding class $y_i \in \{-1, 1\}$, using already trained models $f_A(x_i)$ or $f_B(x_i)$. One can estimate their respective performance on some test data by counting the number of utterances of each possible outcome: either the obtained class corresponds to the desired class, or not. Let $N_{e,A}$ (resp. $N_{e,B}$) be the number of errors of model A (resp. B) and N the total number of test examples; The difference between models A and B can then be written as

$$D = \frac{N_{e,A} - N_{e,B}}{N} . \tag{1}$$

The usual starting point of most statistical tests is to define the so-called *null hypothesis* H_0 which considers that the two models are equivalent, and then verifies how probable this hypothesis is. Hence, assuming that D is an instance of some random variable $\mathbf{D}$ which follows some distribution, we are interested in

$$p(|\mathbf{D}| < |D|) < \alpha \tag{2}$$

where α represents the risk of selecting the *alternate hypothesis* (the two models are different) while the *null hypothesis* is in fact true. This can in general be estimated easily when the distribution of $\mathbf{D}$ is known. In the simplest case, known as the *proportion test*, one assumes (reasonably) that the decision taken by each model on each example can be modeled by a Bernoulli, and further assumes that the errors of the models are independent. This is in general wrong in machine learning since the evaluation sets are the same for both models. When N is large, this leads to estimate $\mathbf{D}$ as a Normal distribution with zero mean and standard deviation σ_D

$$\sigma_D = \sqrt{\frac{2\bar{C}(1-\bar{C})}{N}} \tag{3}$$

where $\bar{C} = \frac{N_{e,A}+N_{e,B}}{2N}$ is the average classification error. In order to get rid of the wrong independence assumption between the errors of the models, the McNemar test [6] concentrates on examples which were differently classified by the two compared models. Following the notation of [4], let N_{01} be the number of examples misclassified by model A but not by model B and N_{10} the number of examples misclassified by model B but not by model A. It can be shown that the following statistics is approximatively distributed as a χ^2 with 1 degree of freedom:

$$z = \frac{(|N_{01} - N_{10}| - 1)^2}{N_{01} + N_{10}}. \tag{4}$$

More recently, several other statistical tests have been proposed, such as the 5x2cv method [4] or the variance estimate proposed in [8], which both claim to better estimate the distribution of the errors (and hence the confidence on the statistical significance of the results). Note however that these solutions assume that the error of one model is the average of some random variable (the error) estimated on each example. Intuitively, it will thus tend to be Normally distributed as N grows, following the central limit theorem.

2.1 The F_1 Measure

Text categorization is the task of assigning one or several categories, among a predefined set of K categories, to textual documents. As explained in [10], text categorization is usually solved as K 2-class classification problems, in a one-against-the-others approach. In this field two measures are considered of importance:

$$\text{Precision} = \frac{N_{tp}}{N_{tp} + N_{fp}}, \quad \text{and} \quad \text{Recall} = \frac{N_{tp}}{N_{tp} + N_{fn}},$$

where for each category N_{tp} is the number of true positives (documents belonging to the category that were classified as such), N_{fp} the number of false positives (documents out of this category but classified as being part of it) and N_{fn} the number of false negatives (documents from the category classified as out of it). Precision and Recall are effectiveness measures, *i.e.* inside $[0, 1]$ interval, the closer to 1 the better. For each category k, Precision_k measures the proportion of documents of the class among the ones considered as such by the classifier and Recall_k the proportion of documents of the class correctly classified.

To summarize these two values, it is common to consider the so-called F_1 measure [11], often used in domains such as information retrieval, text categorization, or vision processing. F_1 can be described as the inverse of the harmonic mean of Precision and Recall:

$$F_1 = \left(\frac{1}{2}\left[\frac{1}{\text{Recall}} + \frac{1}{\text{Precision}}\right]\right)^{-1} = \frac{2 \cdot \text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}} = \frac{2N_{tp}}{2N_{tp} + N_{fn} + N_{fp}}. \tag{5}$$

Let us consider two models A and B, which achieve a performance measured by $F_{1,A}$ and $F_{1,B}$ respectively. The difference $dF_1 = F_{1,A} - F_{1,B}$ does not fit the assumptions of the tests presented earlier. Indeed, it cannot be decomposed into a sum over the documents of independent random variables, since the numerator and the denominator of dF_1 are non constant sums over documents of independent random variables. For the same reason F_1, while being a proportion, cannot be considered as a random variable following a Normal distribution for which we could easily estimate the variance.

An alternative solution to measure the statistical significance of dF_1 is based on the Bootstrap Percentile Test proposed in [5]. The idea of this test is to approximate the unknown distribution of dF_1 by an estimate based on bootstrap replicates of the data.

2.2 Bootstrap Percentile Test

Given an evaluation set of size N, one draws, *with replacement*, N samples from it. This gives the first bootstrap replicate B_1, over which one can compute the statistics of interest, dF_{1,B_1}. Similarly, one can create as many bootstrap replicates B_n as needed, and for each, compute dF_{1,B_n}. The higher n is, the more precise should be the statistical test. Literature [3] suggests to create at least $\frac{50}{\alpha}$ replicates where α is the level of the test; for the smallest α we considered (0.01), this amounts to 5000 replicates. These 5000 estimates dF_{1,B_i} represent the non-parametric distribution of the random variable $\mathbf{dF_1}$. From it, one can for instance consider an interval $[a, b]$ such that $p(a < \mathbf{dF_1} < b) = 1 - \alpha$ centered around the mean of $p(\mathbf{dF_1})$. If 0 lies outside this interval, one can say that $dF_1 = 0$ is not among the most probable results, and thus reject the null hypothesis.

3 Analysis of Statistical Tests

We report in this section an analysis of the bootstrap percentile test, as well as other more classical statistical tests, based on a real large database. We first describe the database itself and the protocol we used for this analysis, and then provide results and comments.

3.1 Database, Models and Protocol

All the experiments detailed in this paper are based on the very large RCV1 Reuters dataset [9], which contains up to 806,791 documents. We divided it as follows: 798,809 documents were kept aside and any statistics computed over this set D_{true} was considered as being the *truth* (*ie* a very good estimate of the actual value); the remaining 7982 documents were used as a training set D_{tr} (to train models A and B). There was a total of 101 categories and each document was labeled with one or more of these categories.

We first extracted the dictionary from the training set, removed stop-words and applied stemming to it, as normally done in text categorization. Each document was then represented as a bag-of-words using the usual $tfidf$ coding. We trained three different models: a linear Support Vector Machine (SVM), a Gaussian kernel SVM, and a multi-layer perceptron (MLP). There was one model for each category for the SVMs, and a single MLP for the 101 categories. All models were properly tuned using cross-validation on the training set.

Using the notation introduced earlier, we define the following competing hypotheses:
$H_0 : |dF_1| = 0$ and $H_1 : |dF_1| > 0$. We further define the level of the test $\alpha = p(\text{Reject } H_0|H_0)$, where α takes on values 0.01, 0.05 and 0.1. Table 1 summarizes the possible outcomes of a statistical test. With that respect, rejecting H_0 means that one is confident with $(1-\alpha)\cdot 100\%$ that H_0 is really false.

In order to assess the performance of the statistical test on Type I errors[1], we used the following protocol. For each category C_i, when H_0 was verified on D_{true} we sampled S (500) evaluation sets D^s_{te} of N documents, ran the significance test over each D^s_{te} and computed the proportion of sets for which H_0 was rejected. We used this proportion as an estimate of the significance test's probability,

[1]For results related to the power of the test see appendix A

Table 1: Various outcomes of a statistical test, with $\alpha = p$(Type I error).

Truth	Decision: Reject H_0	Decision: Accept H_0
H_0	Type I error	OK
H_1	OK	Type II error

α^{true}, of making a Type I error. When α^{true} is higher than the α fixed by the statistical test, the test underestimates Type I error, which means we should not rely on its decision regarding the superiority of one model over the other. Thus, we consider that the significance test fails. On the contrary, $\alpha^{true} < \alpha$ yields a pessimistic statistical test that decides correctly H_0 more often than predicted.

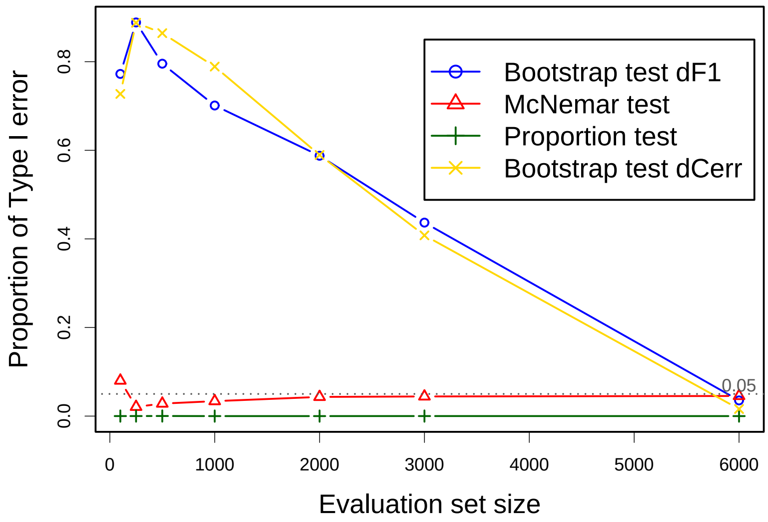
3.2 Summary of Conditions

In order to verify the sensitivity of the analyzed statistical tests to several conditions, we varied the following parameters:

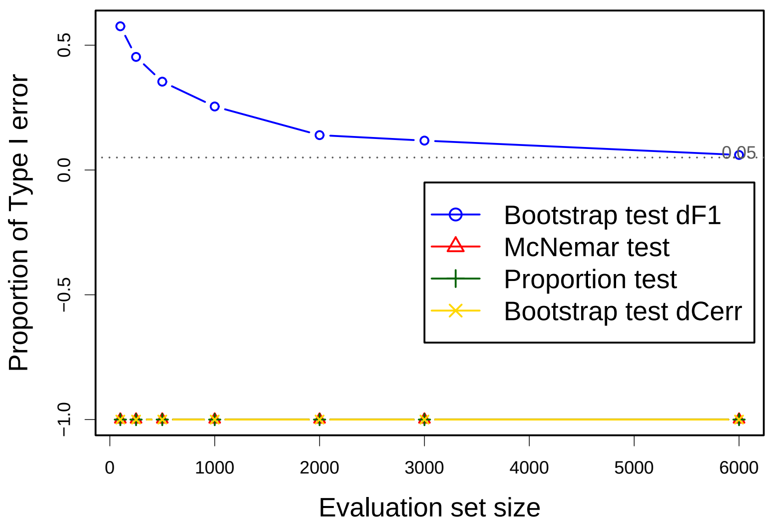
- the value of α: it took on values in $\{0.1, 0.05, 0.01\}$;
- the two compared models: there were three models, two of them were of the same family (SVMs), hence optimizing the same criterion, while the third one was an MLP. Most of the times the two SVMs gave very similar results, (probably because the optimal capacity for this problem was near linear), while the MLP gave poorer results on average. The point here was to verify whether the test was sensitive to the *closeness* of the tested models (although a more formal definition of *closeness* should certainly be devised);
- the evaluation sample size: we varied it from small sizes (100) up to larger sizes (6000) to see the robustness of the statistical test to it;
- the class unbalance: out of the 101 categories of the problem, most of them resulted in highly unbalanced tasks, often with a ratio of 10 to 100 between the two classes. In order to experiment with more balanced tasks, we artificially created *meta-categories*, which were random aggregations of normal categories that tended to be more balanced;
- the tested measure: our initial interest was to directly test dF_1, the difference of F_1, but given poor initial results, we also decided to assess $dCerr$, the difference of classification errors, in order to see whether the tests were sensitive to the measure itself;
- the statistical test: on top of the bootstrap percentile test, we also analyzed the more classical *proportion test* and *McNemar test*, both of them only on $dCerr$ (since they were not adapted to dF_1).

3.3 Results

Figures 1 and 2 summarize the results. All graphs show α^{true}, the number of times the test rejected H_0 while H_0 was true, for a fixed $\alpha = 0.05$, with respect to the sample size, for various statistical tests and tested measures. Figure 1(a) shows the results for balanced data (where the positive and negative examples were approximatively equally present in the evaluation set) when comparing two different models (an SVM and an MLP). Figure 1(b) shows the results for unbalanced data when comparing two different models. Figure 2(a) shows the results for balanced data when comparing two similar models (a linear SVM and a Gaussian SVM) for balanced data, and finally Figure 2(b) shows the results for unbalanced data and two similar models. Note that each point in the graph was computed over a different number of samples, since over the 500×100 only the ones for which H_0 was



(a) Balanced data

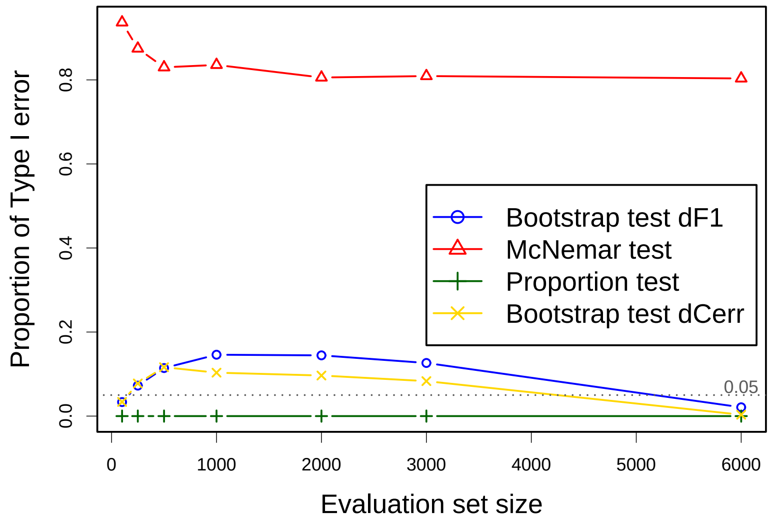


(b) Unbalanced data

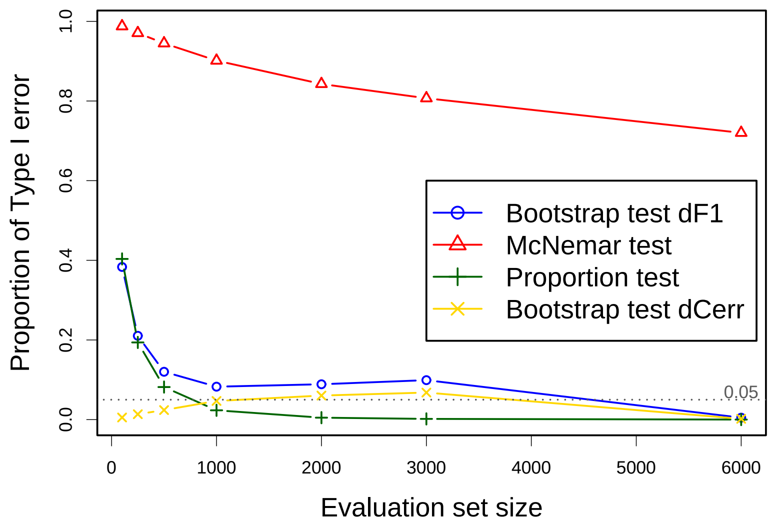
Figure 1: Several statistical tests comparing Linear SVM vs MLP. The proportion of Type I error equals -1, in Figure 1(b), when there was no data to compute the proportion (*ie* H_0 was always false, see appendix B, Fig. 6(b)).

true in D_{true} were taken into account (see appendix B). For each of these graphs, when the curves are over the 0.05 line, that mean that the statistical test is optimistic, while when it is below the line, the statistical test is pessimistic. As already explained, a pessimistic test should be favored whenever possible.

Several interesting conclusions can be drawn from the analysis of these graphs. First of all, as expected, most of the statistical tests are positively influenced by the size of the evaluation set, in the sense that they tend to converge below α for large sample sizes, apart from some exceptions discussed later.



(a) Balanced data



(b) Unbalanced data

Figure 2: Several statistical tests comparing Linear SVM vs RBF SVM

In the cases where the compared models were different, the two bootstrap-based tests (measuring either $dF1$ or $dCerr$) are much more optimistically biased in the balanced data case than the parametric tests. They need very large sample sizes in order to get below the α level. The parametric tests (McNemar and Proportion) both quickly converged to the pessimistic region. Unfortunatelly, in the case of the unbalanced data, H_0 was always false for $dCerr$, thus no analysis can be made regarding the tests based on $dCerr$ values. Comparing the results of the bootstrap test for $dF1$ on balanced and unbalanced data, we can see that this test seems to behave better on the unbalanced data.

The case where the compared models were similar (a linear SVM and a Gaussian SVM) is much more interesting. The first thing to notice is that the McNemar test badly fails in that case. This can be explained by the fact that this test concentrates on examples for which the two models disagree, which can be quite rare for similar models, hence a small number of disagreements may push the statistical test towards concluding that the two models are different while they were not, hence optimistically biasing the results.

Note that most papers studying statistical tests, such as [4] or [8], compare models which are quite different from each other, hence were never exposed to such bad performances. This suggests that there is an intrinsic bias in statistical tests that does not make the independence assumption between the evaluation sets, and which is related to the *closeness* of the compared models. Indeed, the proportion test, which [4] strongly discouraged to use in machine learning, behaves much better in that case.

As for the bootstrap tests, the balanced data case shows a particularity which we could not explain: when the sample size is small, the test deteriorates with the increase of the sample size, while the trend goes back to normal after some threshold size.

To summarize the findings, bootstrap-based statistical tests obtained reasonable performances in most conditions, while the McNemar test failed when the compared models were similar.

4 Conclusion

In this paper, we have analyzed several parametric and non-parametric statistical tests for various conditions often present in machine learning tasks, including the class balancing and the measure to test. We have also varied the *closeness* of the compared models, which has not been done previously in the literature. One surprising conclusion is that when comparing two models which have similar structure or cost functions (such as a linear SVM and a Gaussian SVM), paired statistical tests which do not make wrong independence assumptions, such as the McNemar test, badly fail, to the contrary of other tests, including the simple proportion test.

The starting point of the paper was to verify how non-parametric statistical tests behave when confronted to non-standard measures, such as $dF1$, which could not be assessed by most classical statistical tests. The conclusions were reasonably good with that respect.

It has to be noted that recently, a probabilistic interpretation of F_1 was suggested in [7], and a comparison with bootstrap-based tests should be worthwhile. Note also that in most information retrieval and text categorization tasks, the interesting measure is not simply $dF1$ for each category or query, but some kind of averaging (micro- or macro-), for which a proper statistical test is yet to be devised.

Thanks

We would like to thank Johnny Mariéthoz and Yves Grandvalet for valuable discussions. This work was supported in part by the Swiss NSF through the NCCR on IM2 and in part by the European PASCAL Network of Excellence, IST-2002-506778, through the Swiss OFES.

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A The Power of the Test

In addition to Type I error, it is usual to consider the *power* of a statistical test in order to measure its performance:

$$power = P(RejectH_0|H_1) = 1 - \text{Type II error.}$$

We report in Figures 3 and 4 an estimate of the power of the tests, for the set of conditions defined in Section 3.2. In order to compute this estimate we implemented a protocol similar to the one defined in Section 3.1. For each category C_i, when H_0 was not verified on D_{true} we sampled S (500) evaluation sets D^s_{te} of N documents, ran the significance test over each D^s_{te} and computed the estimate of the power as the proportion of sets for which H_0 was rejected.

B When is H_0 Verified?

As may be noticed in, for example Figure 5(d), most values of dC_{err} over D_{true} (noted dC^*_{err}) range very near 0 without actually being equal to 0. Thus, in the protocol defined in Section 3.1, in order to decided whether or not H_0 was true on D_{true} we proceeded as follows:

Considering a sample of size N, we will say that H_0 is true over D_{true} if $|dM^*| < bound$

where

$$bound = \frac{1}{N} \text{ if } dM^* = dC^*_{err}$$

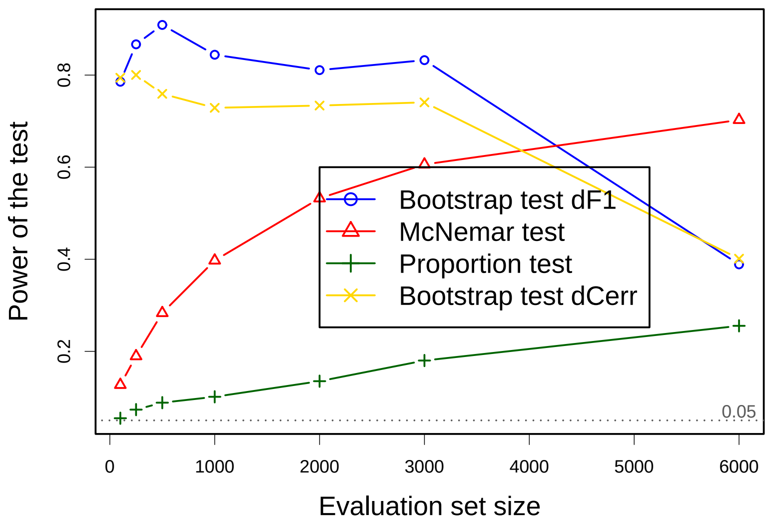
and

$$bound = \frac{n}{N \times n_{pos}} \text{ if } dM^* = dF^*_1$$

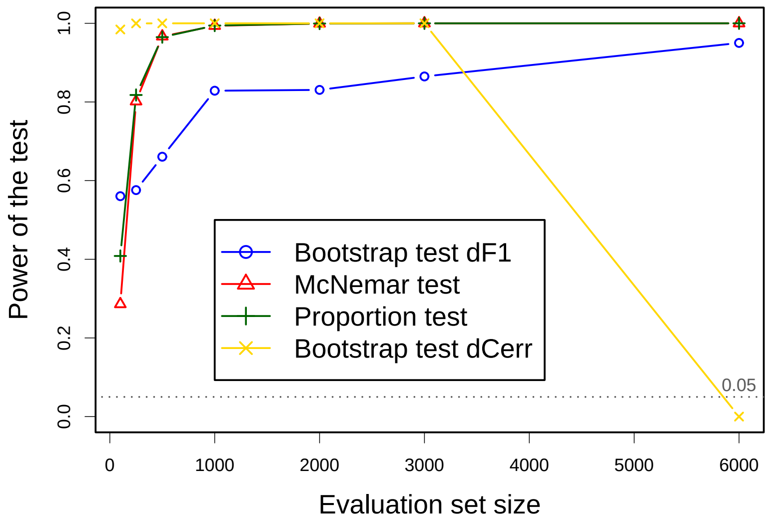
with $n = |D_{true}|$ and n_{pos} being the number of positive examples (documents belonging to the category) in D_{true}.

In the case of $dM^* = dC^*_{err}$, the use of such a bound can be justified by the fact that in a set D^s of size N, H_0 will be verified whenever $|\#error_A - \#error_B| < 1 \Leftrightarrow dC_{err} < \frac{1}{N}$. The justification for $dM^* = dF^*_1$ is quite similar. Given that F_1 is computed at the breakeven point we can say that: $F_1 = \text{Recall} = \frac{N_{tp}}{N_{pos}}$ (see eq. (5)), where N_{pos} is the number of positive examples in D^s. Thus H_0 will be verified in D^s whenever $|N^A_{tp} - N^B_{tp}| < 1 \Leftrightarrow dF^s_1 < \frac{1}{N_{pos}}$. Finally, since we assume that the sample D^s is *i.i.d.* and from the same distribution than D_{true} we have: $\frac{N}{N_{pos}} = \frac{n}{n_{pos}}$.

We report in Figures 6 and 7 the proportion of samples for which H_0 was true in the protocol explained in Section 3.1.

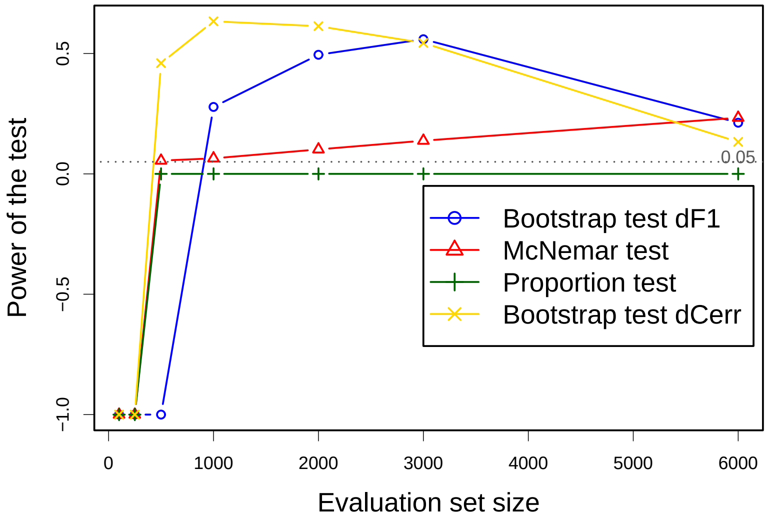


(a) Balanced data

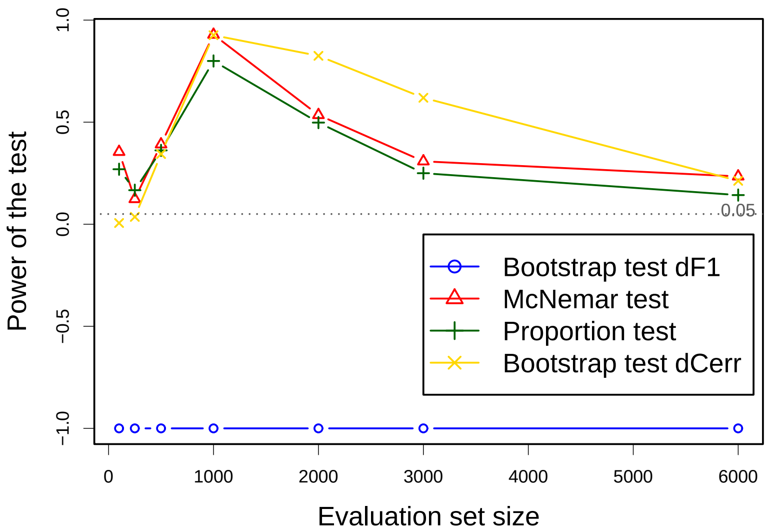


(b) Unbalanced data

Figure 3: Power of several statistical tests comparing Linear SVM vs MLP.

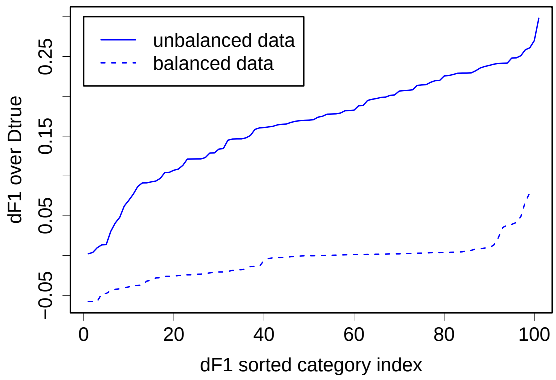


(a) Balanced data

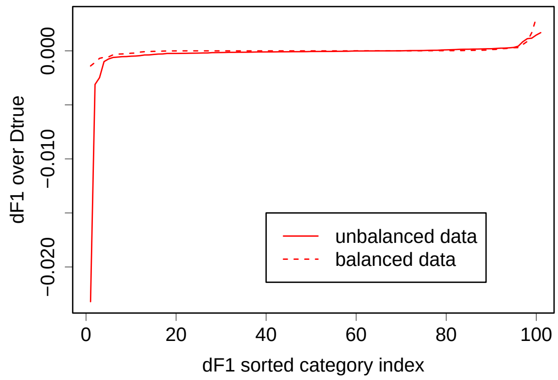


(b) Unbalanced data

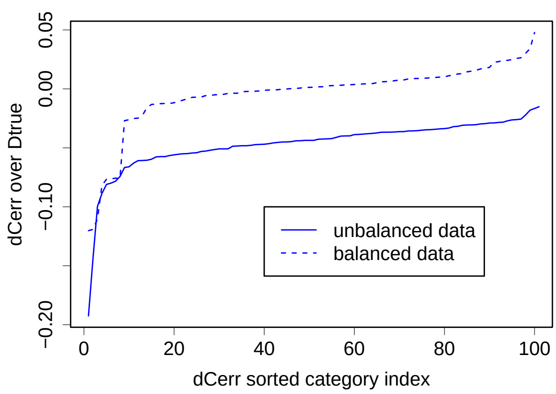
Figure 4: Power of several statistical tests comparing Linear SVM vs RBF SVM. The power equals -1, in Figure 4, when there was not data to compute the proportion (*ie* H_1 was never true, see appendix B, Fig. 7(b)).



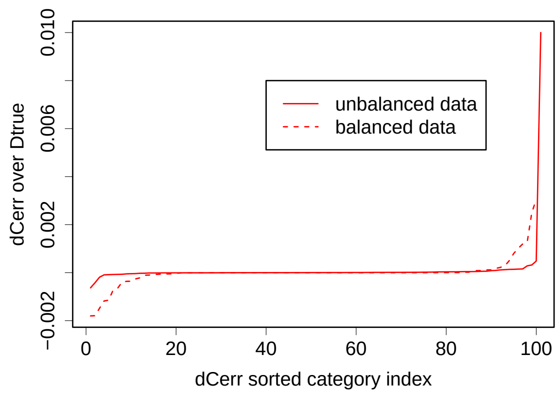
(a) $dF1$ for linear SVM vs MLP



(b) $dF1$ for linear SVM vs RBF SVM

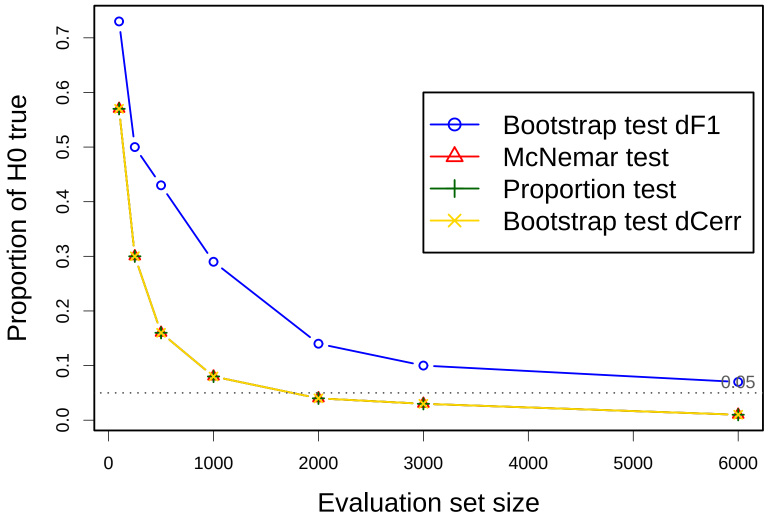


(c) dC_{err} for linear SVM vs MLP

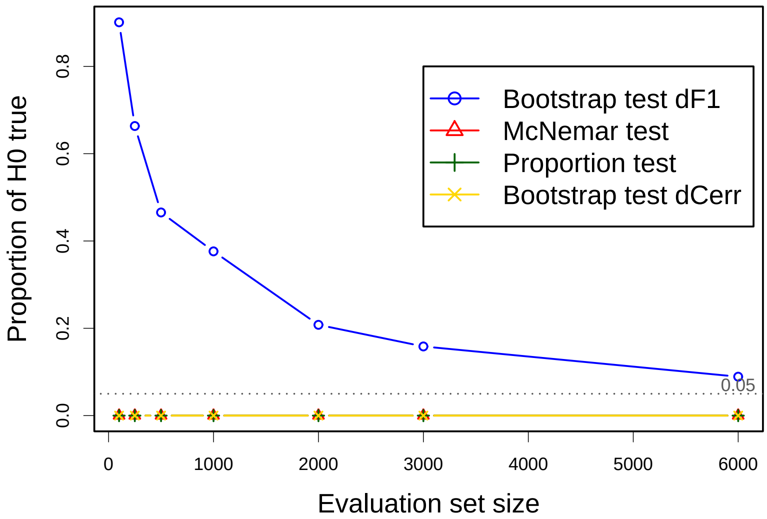


(d) dC_{err} for linear SVM vs RBF SVM

Figure 5: Values of the differences over D_{true}.

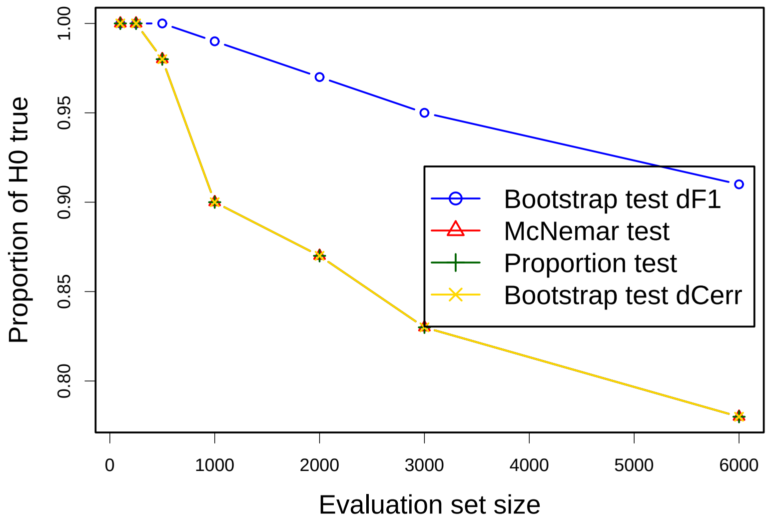


(a) Balanced data

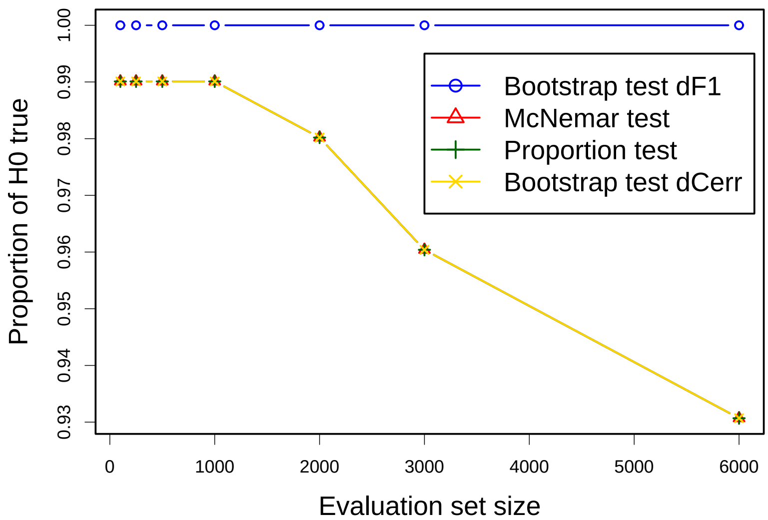


(b) Unbalanced data

Figure 6: Proportion of samples for which H_0 was considered as true in D_{true} for several statistical tests comparing Linear SVM vs MLP.



(a) Balanced data



(b) Unbalanced data

Figure 7: Proportion of samples for which H_0 was considered as true in D_{true} for several statistical tests comparing Linear SVM vs SVM.