AUC: Nonparametric Estimators and Their Smoothness

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Abstract

Nonparametric estimation of a statistic, in general, and of the error rate of a classification rule, in particular, from just one available dataset through resampling is well mathematically founded in the literature using several versions of bootstrap and influence function. This article first provides a concise review of this literature to establish the theoretical framework that we use to construct, in a single coherent framework, nonparametric estimators of the AUC (a two-sample statistic) other than the error rate (a one-sample statistic). In addition, the smoothness of some of these estimators is well investigated and explained. Our experiments show that the behavior of the designed AUC estimators confirms the findings of the literature for the behavior of error rate estimators in many aspects including: the weak correlation between the bootstrap-based estimators and the true conditional AUC; and the comparable accuracy of the different versions of the bootstrap estimators in terms of the RMS with little superiority of the .632+ bootstrap estimator.

Keywords: Statistical Learning, Machine Learning, Bootstrap, Jackknife, Influence Function, Nonparametric Assessment, Error Rate, Receiver Operating Characteristic, ROC, Area Under the Curve, AUC.

1. Introduction

1.1. Formalization and Notation

Consider the binary classification problem, where a classification rule $\eta$ has been trained on the training dataset $t$. This classifier gives a score of $h(x)$ for the predictor $x$, and classifies it to one of the two classes by comparing this score $h(x)$ to a chosen threshold $th$. The observation $x$ belongs to one of the two classes with distributions $F_i$, $i=1,2$. The two error components of this rule are written as:

$$ e_1 = \int_{-\infty}^{th} f_{h}(h(x)|\omega_1) dh(x), \quad (1a) $$

$$ e_2 = \int_{th}^{\infty} f_{h}(h(x)|\omega_2) dh(x). \quad (1b) $$

From the foundations of statistical decision theory, the risk of this rule under the 0-1 loss function, is given by:

$$ R = c_{12} P_1 e_1 + c_{21} P_2 e_2, \quad (2) $$

where, $c_{ij}$ is the cost of classifying an observation as belonging to class $j$ whereas it belongs to class $i$; and $P_i$ is the prior probability of each class, $i=1,2$. The risk (2) is called the “error rate”, $Err$, when putting $c_{12} = c_{21} = 1$.

The risk (or error) is not a sufficient performance measure, since it is function of a single fixed threshold. A more general way to assess a classifier is provided by the Receiver Operating Characteristic (ROC) curve. This is a plot for the two components of error, $e_1$ and $e_2$ under different threshold values. It is conventional in some fields, e.g., medical imaging diagnosis or Automatic Target Recognition (ATR), to refer to $e_1$ as the False Negative Fraction (FNF), and $e_2$ as the False Positive Fraction (FPF). A convention in these fields is to plot the $TPF = 1 - FNF$ vs. the $FPF$. In that case, the farther apart the two distributions of the score function $h(X)$ (under the two classes)from each other, the higher the ROC curve and the larger the area under the curve (AUC). Figure 1 shows ROC curves for two different classifiers. The first one performs better since it has a lower value of $e_2$ at each value of $e_1$. Thus, the first classifier unambiguously separates the two classes better than the second one. Also, the AUC for the first classifier is larger than that for the second one. AUC can be thought of as one summary measure for the ROC curve. Formally the AUC is given by:

$$ AUC = \int_{0}^{1} TPF \, d(FPF). \quad (3) $$
And it can be shown that it is also given by

$$AUC = \Pr[h(x)|\omega_2 < h(x)|\omega_1],$$

which means how the classifier scores for class $\omega_1$ are stochastically larger than those of class $\omega_2$.

If the distributions $F_1$ and $F_2$ are not known, the error rates (1) and the AUC (3)–(4) can be estimated only numerically from a given dataset, called the testing dataset. This is done by assigning equal probability mass for each observation, since this is the Maximum Likelihood Estimation (MLE):

$$\hat{F} : \text{mass } \frac{1}{n} \text{ on } t_i, \ i = 1, \ldots, n,$$

where $n$ is the size of the testing dataset. In this case the nonparametric estimators of (1)–(2) will be given by:

$$\hat{R}(\eta) = \frac{1}{n} \sum_{i=1}^{n} \left( c_{12} I_{h(x_i|\omega_1) < th} + c_{21} I_{h(x_i|\omega_2) > th} \right)$$

$$= \frac{1}{n} \left( c_{21} \hat{e}_1 n_1 + c_{21} \hat{e}_2 n_2 \right)$$

$$= c_{21} \hat{F}_N \hat{P}_1 + c_{21} \hat{F}_F \hat{P}_2.$$ (8)

The indicator function $I_{\text{cond}}$ equals 1 or 0 when the Boolean expression $\text{cond}$ is true or false respectively. The values $n_1$ and $n_2$ are the number of observations in the two classes respectively, and $\hat{P}_1$ and $\hat{P}_2$ are the estimated a priori probabilities for each class.

The two components, $1 - \hat{F}_N$ and $\hat{F}_F$ give one point on the empirical (estimated) ROC curve for a particular threshold value. Then all possible thresholds, between successive scores, are considered in turn. At each threshold value a point on the ROC curve is calculated. Then the population AUC (3) can be estimated from the empirical ROC curve using the trapezoidal rule:

$$\hat{AUC} = \frac{1}{2} \sum_{i=2}^{n_{th}} (FNF_i - FNF_{i-1}) (TPF_i + TPF_{i-1}),$$

where $n_{th}$ is the number of threshold values taken over the dataset. On the other hand, Mann-Whitney statistic—which is another form of the Wilcoxon rank-sum test (Hájek et al., 1999, Ch.4)—defined by:

$$\hat{AUC} = \frac{1}{n_1 n_2} \sum_{j=1}^{n_2} \sum_{i=1}^{n_1} \psi\left(h(x_i|\omega_1), h(x_j|\omega_2)\right),$$

$$\psi(a, b) = \begin{cases} 
1 & a > b \\
1/2 & a = b \\
0 & a < b 
\end{cases}$$

is the Uniform Minimum Variance Unbiased Estimator (UMVUE) for the probability (4). It is easy to show that the AUC estimators (9) and (10) are identical, exactly as their estimands (3) and (4) are.

It is worth mentioning that each of the error estimators $\hat{e}_1$ and $\hat{e}_2$ in (6) is called one-sample statistic since its kernel
1.2. Motivation

The simple nonparametric estimators of the error rate (6) and the AUC (10) are obtained from a single testing dataset as mentioned above. This is one source of variability (or uncertainty). Another source of variability is the variation of the training set \( t \) on which the classifier my train. We should not only be interested in these estimators but also in their mean and variance where the source of randomness is from both the training and testing sets. The way we make up this testing dataset, and hence obtain these estimators and their mean and variance, defines two paradigms. In Paradigm I, we only have one dataset from which we have to make up a training dataset and a testing dataset using one of the resampling techniques. In each resampling iteration we get a training and a testing set. In Paradigm II, as may be imposed by some regulatory agencies, e.g., the FDA, it is mandated that there is a sequestered testing dataset that is never available even for resampling but for just onetime final testing. The theory of assessing classifiers in terms of the AUC under this paradigm is addressed in our work Yousef et al. (2006) and then elaborated in Chen et al. (2012). However, under Paradigm I the theory of assessing classifiers in terms of the error rate is fully accounted mainly in the work of Efron (Efron and Tibshirani, 1997, 1993; Efron, 1983) and others as will be reviewed in Section 3. The role of the present article is to extend this work to account for assessing classifiers under Paradigm I but in terms of the AUC, a two-sample statistic, as opposed to the error rate, a one-sample statistic.

1.3. Manuscript Roadmap

The rest of the article is organized as follows. Section 2 paves the road to the article by reviewing the nonparametric estimators for estimating the mean and variance of one-sample statistics, including the preliminaries of bootstraps and influence function. This section is a very concise review mainly of the work done in Efron and Tibshirani (1993); Hampel (1974); Huber (1996). Section 3 switches gears and reviews the nonparametric estimators that estimate the mean and variance of a special kind of statistics, i.e., the error rate of classification rules. This section is a concise review of the work done mainly in Efron and Tibshirani (1997). Section 4 is the main contribution of the present article that extends the nonparametric estimators that estimate the error rate, a one-sample statistic, to estimate the AUC, a two-sample statistic. It does so by providing theoretical parallelism between the two sets of estimators and showing that the extension is rigorous and not just an ad-hoc application. In addition, it explains and illustrates experimentally the concept of smoothness of some of these estimators and justifies the use of the leave-pair-out estimator for the AUC. Section 5 provides experiments and results that illustrate the accuracy of the nonparametric estimators of the AUC designed in the preceding section and compare the results to those obtained earlier in the literature for the same estimators when they estimated the error rate.

2. Review of Nonparametric Methods for Estimating the Bias and Variance of a Statistic

Assume that there is a statistic \( s \) that is a function of a dataset \( x: \{x_i, i = 1, 2, \ldots, n\} \), where \( x_i \sim \text{i.i.d. } F \). The statistic \( s \) is now a random variable and its variability comes from the variability of \( x_i \). Assume that this statistic is used to estimate a real-valued parameter \( \theta = f(F) \). Then \( \hat{\theta} = s(x) \) has expected value \( E[s(x)] \) and variance \( \text{Var}[s(x)] \). The mean square error of the estimator \( \hat{\theta} \) is defined as:

\[
MSE_{\hat{\theta}} = E[(\hat{\theta} - \theta)^2].
\]  

(12)

The bias of the estimator \( \hat{\theta} = s(x) \) is defined by the difference between the true value of the parameter and the expectation of the estimator, i.e.,

\[
bias_F = bias_F(\hat{\theta}, \theta) = E_F[s(x)] - f(F).
\]

(13)

Then the MSE in (12) can be rewritten as:

\[
MSE_{\hat{\theta}} = bias_F^2(\hat{\theta}) + \text{Var}[\hat{\theta}].
\]

(14)

A critical question is whether the bias and variance of the statistic \( s \) in (14) may be estimated from the available dataset?

2.1. Bootstrap Estimate

The bootstrap was introduced by Efron (1979) to estimate the standard error of a statistic. The bootstrap mechanism is implemented by treating the current dataset \( x \) as a representation for the population distribution \( F \); i.e., approximating the distribution \( F \) by the MLE defined in (5). Then \( B \) bootstrap samples are drawn from that empirical distribution. Each bootstrap replicate is of size \( n \), the same size as \( x \), and is obtained by sampling with replacement. Then in a bootstrap replicate some case \( x_{ij} \), in general, will appear more than once at the expense of another \( x_{ij} \) that will not appear. The original dataset will be treated now as the population, and the replicates will be treated as samples from the population. This situation is illustrated inFigure 2. Therefore, the bootstrap estimate of bias is defined to be:
Figure 2: Bootstrap mechanism: \( B \) bootstrap replicates are withdrawn from the original sample. From each replicate the statistic is calculated.

\[
\hat{\text{bias}}_{\hat{F}}(\hat{\theta}) = \hat{\theta}^* - \hat{\theta}, \tag{15}
\]

\[
\hat{\theta}^* = \frac{1}{B} \sum_{b=1}^{B} \hat{\theta}^{*b}, \tag{16}
\]

\[
\hat{\theta}^{*b} = s(x^{*b}), \tag{17}
\]

\[
\hat{\theta} = s(x). \tag{18}
\]

The bootstrap estimate of standard error of the statistic \( \hat{\theta}(x) \) is defined by:

\[
\hat{SE}_{B} = \left\{ \frac{1}{B} \sum_{b=1}^{B} (\hat{\theta}^{*b} - \hat{\theta}^*)^2 / (B - 1) \right\}^{1/2}. \tag{19}
\]

Either in estimating the bias or the standard error, the larger the number of bootstraps the closer the estimate to the asymptotic value. Said differently:

\[
\lim_{B \to \infty} \hat{SE}_{B}(\hat{\theta}^*) = SE_{\hat{F}}(\hat{\theta}^*). \tag{20}
\]

For more details and some examples the reader is referred to Efron and Tibshirani (1993, Ch. 6, 7, and 10).

2.2. Jackknife Estimate

Instead of replicating from the original dataset, a new set \( x_{(i)} = (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n) \) is created by removing the case \( x_i \) from the dataset. Then the jackknife samples are defined by:

\[
x_{(i)} = (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n), \quad i = 1, \ldots, n, \tag{21}
\]

and the \( n \)-jackknife replications of the statistic \( \hat{\theta} \) are:

\[
\hat{\theta}_{(i)} = s(x_{(i)}), \quad i = 1, \ldots, n. \tag{22}
\]
The jackknife estimates of bias and standard error are defined by:

\[
\text{bias}_{\text{jack}} = (n-1)(\hat{\theta}(\cdot) - \hat{\theta}), \quad (23)
\]

\[
\hat{SE}_{\text{jack}} = \left[ \frac{n-1}{n} \sum_{i=1}^{n} (\hat{\theta}(\cdot) - \hat{\theta}(\cdot))^2 \right]^{1/2}, \quad (24)
\]

\[
\hat{\theta}(\cdot) = \frac{1}{n} \sum_{i=1}^{n} \hat{\theta}_i. \quad (25)
\]

For motivation behind the factors \((n-1)\) and \((n-1)/n\) in (23) see (Efron and Tibshirani, 1993, Ch. 11). The jackknife estimate of variance is discussed in detail in Efron (1981) and Efron and Stein (1981).

2.3. Bootstrap vs. Jackknife

Usually it requires up to 200 bootstraps to yield acceptable bootstrap estimates (in special situations like estimating the uncertainty in classifier performance it may take up to thousands of bootstraps). Hence, this requires calculating the statistic \(\hat{\theta}\) the same number of times \(B\). In the case of the jackknife, it requires only \(n\) calculations as shown in (22). If the sample size is smaller than the required number of bootstraps, the jackknife is more economical in terms of computational cost.

In terms of accuracy, the jackknife can be seen to be an approximation to the bootstrap when estimating the standard error of a statistic; see Efron and Tibshirani (1993, Ch. 20). Thus, if the statistic is linear they almost give the same result (The bootstrap gives the jackknife estimate multiplied by \((n-1)/n\)^{1/2}. A statistic \(s(x)\) is said to be linear if:

\[
s(x) = \mu + \frac{1}{n} \sum_{i=1}^{n} \alpha(x_i), \quad (26)
\]

where \(\mu\) is a constant and \(\alpha(\cdot)\) is a function. This also can be viewed as having one data point at a time in the argument of the function \(\alpha\). Similarly, the jackknife can be seen as an approximation to the bootstrap when estimating the bias. If the statistic is quadratic, they almost agree except in a normalizing factor. A statistic \(s(x)\) is quadratic if:

\[
s(x) = \mu + \frac{1}{n} \sum_{1 \leq i \leq n} \alpha(x_i) + \frac{1}{n^2} \sum_{1 \leq i < j \leq n} \beta(x_i, x_j). \quad (27)
\]

An in-depth treatment of the bootstrap and jackknife and their relation to each other in mathematical detail is provided by Efron (1982, Ch. 1-5).

If the statistic is not smooth the jackknife will fail. Informally speaking, a statistic is said to be smooth if a small change in the data leads to a small change in the statistic. An example of a non-smooth statistic is the median. If the sample cases are ranked and the median is calculated, it will not change when a sample case changes unless this sample case bypasses the median value. An example of a smooth statistic is the sample mean. We will provide a deeper explanation to the smoothness issue, supported with experiments, in Section 4.2.

2.4. Influence Function, Infinitesimal Jackknife, and Estimate of Variance

The infinitesimal jackknife was introduced by Jaeckel (1972). The concept of the influence curve was introduced later by Hampel (1974). In the present context and for pedagogical purposes, the influence curve will be explained before the infinitesimal jackknife, since the former can be understood as the basis for the latter.

Following Hampel (1974), let \(\mathcal{X}\) be the real line and \(s\) be a real-valued functional defined on the distribution \(F\) which is defined on \(\mathcal{X}\). The distribution \(F\) can be perturbed by adding some probability measure (mass) on a point \(x\). This should be balanced by a decrement in \(F\) elsewhere, resulting in a new probability distribution \(G_{\varepsilon,x}\) defined by:

\[
G_{\varepsilon,x} = (1 - \varepsilon)F + \varepsilon \delta_x, \quad x \in \mathcal{X}. \quad (28)
\]

Then, the influence curve \(IC_{s,F}(\cdot)\) is defined by:

\[
IC_{s,F}(x) = \lim_{\varepsilon \to 0^+} \frac{s((1 - \varepsilon)F + \varepsilon \delta_x) - s(F)}{\varepsilon}. \quad (29)
\]

It should be noted that \(F\) does not have to be a discrete distribution. A simple example of applying the influence curve concept is to consider the expectation \(s = \int x \, dF(x) = \mu\). Substituting back in (29) gives:

\[
IC_{s,F}(x) = x - \mu. \quad (30)
\]

The meaning of this formula is the following: the rate of change of the functional \(s\) with the probability measure at a point \(x\) is \(x - \mu\). This is how the point \(x\) influences the function \(s\).
The influence curve can be used to linearly approximate a functional \( s \); this is similar to taking up to only the first-order term in a Taylor series expansion. Assume that there is a distribution \( G \) near to the distribution \( F \); then under some regularity conditions (see, e.g., Huber, 1996, Ch. 2) a functional \( s \) can be approximated as:

\[
s(G) \approx s(F) + \int IC_{s,F}(x) \, dG(x). \tag{31}
\]

The residual error can be neglected since it is of a small order in probability. Some properties of (31) are:

\[
\int IC_{T,F}(x) \, dF(x) = 0, \tag{32}
\]

and the asymptotic variance of \( s(F) \) under \( F \), following from (32), is given by:

\[
\text{Var}_F[s(F)] = \int \{IC_{T,F}(x)\}^2 \, dF(x), \tag{33}
\]

which can be considered as an approximation to the variance under a distribution \( G \) near to \( F \). Now, assume that the functional \( s \) is a functional statistic in the dataset \( \mathbf{x} = \{x_i : x_i \sim F, i = 1, 2, \ldots, n\} \). In that case the influence curve (29) is defined for each sample case \( x_i \), under the true distribution \( F \) as:

\[
U_i(s,F) = \lim_{\varepsilon \to 0} \frac{s(F_{\varepsilon,i}) - s(F)}{\varepsilon} = \left. \frac{\partial s(F_{\varepsilon,i})}{\partial \varepsilon} \right|_{\varepsilon=0}, \tag{34}
\]

where \( F_{\varepsilon,i} \) is the distribution under the perturbation at observation \( x_i \). In the sequel, (34) will be called the influence function. If the distribution \( F \) is not known, the MLE \( \hat{F} \) of the distribution \( F \) is given by (5), and as an approximation \( \hat{F} \) may substitute for \( F \) in (34). The result may then be called the empirical influence function (Mallows, 1974), or infinitesimal jackknife (Jaeckel, 1972). In such an approximation, the perturbation defined in (28) can be rewritten as:

\[
\hat{F}_{\varepsilon,i} = (1 - \varepsilon)\hat{F} + \varepsilon \delta_{x_i}, \quad x_i \in \mathbf{x}, \quad i = 1, \ldots, n. \tag{35}
\]

This kind of perturbation is illustrated in Figure 3. It will often be useful to write the probability mass function of (35) as:

\[
\hat{f}_{\varepsilon,i}(x_j) = \left\{ \begin{array}{ll}
\frac{1 - \varepsilon}{n} + \varepsilon & j = i \\
\frac{1 - \varepsilon}{n} & j \neq i
\end{array} \right.. \tag{36}
\]

Substituting \( \hat{F} \) for \( G \) in (31) and combining the result with (34) gives the influence-function approximation for any functional statistic under the empirical distribution \( \hat{F} \). The result is:

\[
s(\hat{F}) = s(F) + \frac{1}{n} \sum_{i=1}^{n} U_i(s,F) + O_p(n^{-1}) \tag{37}
\]

\[
\approx s(F) + \frac{1}{n} \sum_{i=1}^{n} U_i(s,F). \tag{38}
\]

The term \( O_p(n^{-1}) \) reads “big-O of order 1/n in probability”. In general, \( U_n = O_p(d_n) \) if \( U_n / d_n \) is bounded in probability,
over-designing a classifier to minimize the apparent error is not the goal. The goal is to minimize the true error rate (41). The asymptotic variance expressed in (33) can be given for $s$ i.e., $\Pr\{s(U) < k_2\} > 1 - \varepsilon \forall \varepsilon > 0$. This concept can be found in Barndorff-Nielsen and Cox (1989, Ch. 2). Then the asymptotic variance expressed in (33) can be given for $s(F)$ by:

$$\text{Var}_F[s] = \frac{1}{n} E_F \left[ U^2(x_i, F) \right],$$

which can be approximated under the empirical distribution $\hat{F}$ to give the nonparametric estimate of the variance for a statistic $s$ by:

$$\widehat{\text{Var}}_F[s] = \frac{1}{n^2} \sum_{i=1}^n U_i^2(x_i, \hat{F}).$$

It is important to state here that $s$ should be a functional in $\hat{F}$ that is an approximation to $F$, as was initially assumed in (29). If for example the value of the statistic $s$ changes if every sample case $x_i$ is duplicated, i.e., repeated twice, this is not a functional statistic. An example of a functional statistic is the biased version of the variance estimate (29). If for example the value of the statistic $s$ is duplicated, i.e., repeated twice, this is not a functional statistic. Generally, any approximation $s(\hat{F})$ to the functional $s(F)$, by approximating $F$ by the MLE $\hat{F}$, obviously will be functional. In such a case the statistic $s(\hat{F})$ is called the plug-in estimate of the functional $s(F)$. Moreover, the influence function method for variance estimation is applicable only to those functional statistics whose derivative (34) exists. If that derivative exists, the statistic is called a smooth statistic; i.e., a small change in the dataset leads a small change in the statistic. For instance, the median is a functional statistic in the sense that duplicating any sample case will result in the same value of the median. On the other hand it is not smooth as described at the end of Section 2.3. A key reference for the influence function is Hampel (1986).

A very interesting case arises from (36) if $-1/(n + 1)$ is substituted for $\varepsilon$. In this case the new probability mass assigned to the point $x_j = 1$ in (36) will be zero. This value of $\varepsilon$ simply generates the jackknife estimate discussed in Section 2.2 where the whole point is removed from the dataset.

3. Review of Nonparametric Methods for Estimating the Error Rate of a Classification Rule

In the previous section the statistic, or generally speaking the functional, was a function of just one dataset. For a non-fixed design, i.e., when the predictors for the testing set do not have to be the same as the predictors of the training set, a slight clarification for the previous notations is needed. The classification rule trained on the training dataset $t$ will be denoted as $\eta_t$. Any new observation that does not belong to $t$ will be denoted by $t_0 \equiv (x_o, y_o)$. Therefore the loss due to classification is given by $L(y_o, \eta_t(x_o))$. Any performance measure conditional on that training dataset will be similarly subscripted. Thus, the risk (2) and the error rate whose two components are (1), should be denoted by $R_t$ and $Err_t$, respectively. In the sequel, for simplicity and without loss in generality, the 0-1 loss function will be used. In such a case the conditional error rate will be given by:

$$Err_t = E_{0,F} \left[ L(y_o, \eta_t(x_o)) \right], \quad (x_o, y_o) \sim F.$$

The expectation $E_{0,F}$ is subscripted so to emphasize that it is taken over the observations $t_0 \notin t$. If the performance is measured in terms of the error rate and we are interested in the mean performance, not the conditional one, then it is given by:

$$Err = E_t[Err_t],$$

where $E_t$ is the expectation over the training set $t$, which would be the same if we had written $E_F$; for notation clarity the former is chosen.

Consider a classification rule $\eta_t$ already trained on a training dataset $t$. A natural next question is, given that there is just a single dataset available, how to use this dataset in assessing the classifier performance as well? Said differently, how should one estimate, using only the available dataset, the classification performance of a classification rule in predicting new observations; these observations are different from those on which the rule was trained. In this section, the principal methods in the literature for estimating the mean and variance of the error rate of a classification rule are reviewed and summarized.

3.1. Apparent Error

The apparent error is the error of the fitted model when it is tested on the same training data. Of course it is downward biased with respect to the true error rate since it results from testing on the same information used in training (Efron, 1986). The apparent error is defined by:

$$\text{Err}_t = E_F L(y, \eta_t(x)), (x, y) \in t$$

$$= \frac{1}{n} \sum_{i=1}^n \left( I_{h_1(x_i|\omega_1) < t} + I_{h_1(x_i|\omega_2) > t} \right).$$

Over-designing a classifier to minimize the apparent error is not the goal. The goal is to minimize the true error rate (41).
3.2. Cross Validation (CV)

The basic concept of Cross Validation (CV) has been proposed in different articles since the mid-1930s. The concept simply leans on splitting the data into two parts; the first part is used in design without any involvement of the second part. Then the second part is used to test the designed procedure; this is to test how the designed procedure will behave for new datasets. Stone (1974) is a key reference for CV that proposes different criteria for optimization.

CV can be used to assess the prediction error of a model or in model selection. In this section the former is discussed. The true error rate in (41) is the expected error rate for a classification rule if tested on the population, conditional on a particular training dataset \( t \). This performance measure can be approximated by leave-one-out cross-validation (LOOCV) by:

\[
\bar{\text{Err}}_{t}^{\text{cv}} = \frac{1}{n} \sum_{i=1}^{n} L(y_{i}, \eta_{t^{\text{cv}}}(x_{i})), \quad (x_{i}, y_{i}) \in t. \tag{45}
\]

This is done by training the classification rule on the dataset \( t^{(i)} \) that does not include the case \( t_{i} \); then testing the trained rule on that omitted case. This proceeds in “round-robin” fashion until all cases have contributed one at a time to the error rate. There is a hidden assumption in this mechanism: the training set \( t \) will not change very much by omitting a single case. Therefore, testing on the omitted points one at a time accounts for testing approximately the same trained rule on \( n \) new cases, all different from each other and different from those the classifier has been trained on. Besides this LOOCV, there are other versions named \( k \)-fold (or leave-\( n/k \)-out). In such versions the whole dataset is split into \( k \) roughly equally-sized subsets, each of which contains approximately \( n/k \) observations. The classifier is trained on \( k-1 \) subsets and tested on the left-out one; hence we have \( k \) iterations.

It is of interest to assess this estimator to see if it estimates the conditional true error with small MSE: \( E \left[ \bar{\text{Err}}_{t}^{\text{cv}} - \text{Err}_{t} \right]^{2} \). Many simulation results, e.g., Efron (1983), show that there is only a very weak correlation between the cross validation estimator and the conditional true error rate \( \bar{\text{Err}}_{t} \). This issue is discussed in mathematical detail in the excellent paper by Zhang (1995). Other estimators to be discussed below are shown to have this same attribute.

3.3. Bootstrap Methods for Error Rate Estimation

The prediction error in (41) is a function of the training dataset \( t \) and the testing population \( F \). Bootstrap estimation can be implemented here by treating the empirical distribution \( \hat{F} \) as an approximation to the actual population distribution \( F \). By replicating from that distribution one can simulate the case of many training datasets \( t_{b}, b = 1, \ldots, B \), the total number of bootstraps. For every replicated training dataset the classifier will be trained and then tested on the original dataset \( t \). This is the Simple Bootstrap (SB) estimator approach (Efron and Tibshirani, 1993, Sec. 17.6) that is defined formally by:

\[
\bar{\text{Err}}_{t}^{\text{SB}} = E_{*} \sum_{i=1}^{n} L(y_{i}, \eta_{t^{\text{SB}}}(x_{i}))/n, \quad \hat{F} \rightarrow t^{*}. \tag{46}
\]

It should be noted that this estimator no longer estimates the true error rate (41) because the expectation taken over the bootstraps mimics an expectation taken over the population of trainers, i.e., it is not conditional on a particular training set. Rather, the estimator (46) estimates the expected performance of the classifier \( E_{F} \bar{\text{Err}}_{t} \), which is a constant performance measure, not a random variable any more. For a finite number of bootstraps the expectation (46) can be approximated by:

\[
\bar{\text{Err}}_{t}^{\text{SB}} = \frac{1}{B} \sum_{b=1}^{B} \sum_{i=1}^{n} L(y_{i}, \eta_{t^{\text{SB}}}(x_{i}))/n. \tag{47}
\]

3.3.1. Leave-One-Out Bootstrap (LOOB)

The previous estimator is obviously biased since the original dataset \( t \) used for testing includes part of the training data in every bootstrap replicate. Efron (1983) proposed that, after training the classifier on every bootstrap replicate, it is tested on those cases in the set \( t \) that are not included in the training; this concept can be developed as follows. Equation (47) can be rewritten by interchanging the order of the double summation to give:

\[
\bar{\text{Err}}_{t}^{\text{SB}} = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{1}{B} \sum_{b=1}^{B} L(y_{i}, \eta_{t^{\text{SB}}}(x_{i}))/B \right). \tag{48}
\]

This equation is formally identical to (47) but it expresses a different mechanism for evaluating the same quantity. It says that, for a given point, the average performance over the bootstrap replicates is calculated; then this performance is averaged over all the \( n \) cases. Now, if every case \( t_{i} \) is tested only from those bootstraps that did not include it in the training, a slight modification of the previous expression yields the leave-one-out bootstrap (LOOB) estimator:

\[
\bar{\text{Err}}_{t}^{\text{LOOB}} = \frac{1}{n} \sum_{i=1}^{n} \left[ \frac{1}{B} \sum_{b=1}^{B} I_{b}^{i} L(y_{i}, \eta_{t^{\text{LOOB}}}(x_{i}))/B \sum_{b=1}^{B} I_{b}^{i} \right], \tag{49}
\]

where the indicator function \( I_{b}^{i} \) equals one when the case \( t_{i} \) is not included in the training replicate \( b \), and zero otherwise. To simplify notation, the error \( L(y_{i}, \eta_{t^{\text{LOOB}}}(x_{i})) \) may be denoted by \( I_{i}^{b} \). Efron and Tibshirani (1997) emphasized a critical
point about the difference between this bootstrap estimator and LOOCV. The CV tests on a given sample case $t_i$, having been trained just once on the remaining dataset. By contrast, the LOOB tests on a given sample case $t_i$ using a large number of classifiers that result from a large number of bootstrap replicates that do not contain that sample. This results in a smoothed cross-validation-like estimator. In the present article, we explain and elaborate on the smoothness property (Section 4.2).

### 3.3.2. The Refined Bootstrap (RB)

The SB and the LOOB, from their definitions, look like designed to estimate the mean true error rate for a classifier. This mean is with respect to the population of all training datasets. For estimating the true error rate of a classifier, conditional on a particular training dataset, Efron (1983) proposed to correct for the downward biased estimator $\overline{E_{\text{err}}}$, Since the true error rate $E_{\text{err}}$ can be written as $\overline{E_{\text{err}}}$, then it can be approximated by $\overline{E_{\text{err}}} + E_F(\overline{E_{\text{err}}} - \overline{E_{\text{err}}})$. The term $\overline{E_{\text{err}}} - \overline{E_{\text{err}}}$ is called the optimism. The expectation of the optimism can be approximated over the bootstrap population. Finally the refined bootstrap approach, as named in Efron and Tibshirani (1993, Sec. 17.6), gives the estimator:

$$\overline{E_{\text{err}}}^{RF} = \overline{E_{\text{err}}} + E_{F}(\overline{E_{\text{err}}} - \overline{E_{\text{err}}})$$

(50)

where $E_{err}^{RF}$ represents the error rate obtained from training the classifier on the bootstrap replicate $t^*$ and testing on the empirical distribution $F$. This can be approximated for a limited number of bootstraps by:

$$\overline{E_{\text{err}}}^{RF} = \overline{E_{\text{err}}} + \frac{1}{B} \sum_{b=1}^{B} \left\{ \sum_{i=1}^{n} L(y_i, \eta^{b}(x_i)) / n - \sum_{i=1}^{n} L(y_i^*, \eta^{b}(x_i^*)) / n \right\}$$

(51)

### 3.3.3. The 0.632 Bootstrap

If the concept used in developing the LOOB estimator, i.e., testing on cases not included in training, is used again in estimating the optimism described above, this gives the 0.632 bootstrap estimator. Since the probability of including a case $t_i$ in the bootstrap $t_i^{*b}$ is given by:

$$\Pr(t_i \in t_i^{*b}) = 1 - (1 - 1/n)^n$$

(52)

$$\approx 1 - e^{-1} = 0.632,$$

(53)

the effective number of sample cases contributing to a bootstrap replicate is approximately 0.632 of the size of the training dataset. Efron (1983) introduced the concept of a distance between a point and a sample set in terms of a probability. Having trained on a bootstrap replicate, testing on those cases in the original dataset not included in the bootstrap replicate accounts for testing on a set far from the training one, i.e., the bootstrap replicate. This is because every sample case in the testing set has zero probability of belonging to the training set, i.e., very distant from the training set. This is a reason for why the LOOB is upward biased estimator. Efron (1983) showed roughly that:

$$E_F \left\{ \overline{E_{\text{err}}} - \overline{E_{\text{err}}} \right\} \approx 0.632 E_F \left\{ \overline{E_{\text{err}}} - \overline{E_{\text{err}}} \right\}$$

(54)

Substituting back in (50) gives the 0.632 estimator:

$$\overline{E_{\text{err}}}^{(632)} = .368 \overline{E_{\text{err}}} + .632 \overline{E_{\text{err}}}$$

(55)

The proof of the above results can be found in Efron (1983) and Efron and Tibshirani (1993, Sec. 6).

The motivation behind this estimator as stated earlier is to correct for the downward biased apparent error by adding a piece of the upward biased LOOB estimator. But an increase in variance should be expected as a result of adding this piece of the relatively variable apparent error. Moreover, this new estimator is no longer smooth since the apparent error itself is unsmooth.

### 3.3.4. The 0.632+ Bootstrap Estimator

The .632 estimator reduces the bias of the apparent error. But for over-trained classifiers, i.e., those whose apparent error tends to be zero, the .632 estimator is still downward biased. Breiman et al. (1984) provided the example of an over-fitted rule, like 1-nearest neighbor where the apparent error is zero. If, however, the class labels are assigned randomly to the predictor. Then for a training sample $t$, $\gamma$ can be estimated by:

$$\gamma = E_{oF_{ind}} \left[ L(y_0, \eta(x_0)) \right]$$

(56)

where $F_{ind}$ means that $x_0$ and $y_0$ are distributed marginally as $F$ but they are independent. Or said differently, the label is assigned randomly to the predictor. Then for a training sample $t$, $\gamma$ can be estimated by:

$$\hat{\gamma} = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} L(y_i, \eta(x_j)) / n^2$$

(57)
This means that the $n$ predictors have been permuted with the $n$ responses to produce $n^2$ non-informative cases. In the special case of binary classification, let $\hat{p}_1$ be the proportion of the response classified as belonging to class 1. Also, let $\hat{q}_1$ be the proportion of the responses classified as belonging to class 1. Then (57) reduces to:

$$\hat{\gamma} = \hat{p}_1 (1 - \hat{q}_1) + (1 - \hat{p}_1) \hat{q}_1.$$  

(58)

Also define the relative overfitting rate:

$$\hat{R} = \frac{\overline{Err}_t^{(1)} - \overline{Err}_t}{\hat{\gamma} - \overline{Err}_t}.$$  

(59)

Efron and Tibshirani (1997) showed that the bias of the .632 estimator for the case of over-fitted classifiers is alleviated by using a renormalized version of that estimator:

$$\overline{Err}_t^{(632+)} = (1 - \hat{w}) \overline{Err}_t + \hat{w} \overline{Err}_t^{(1)}.$$  

(60)

$$\hat{w} = \frac{.632}{1 - .368 \hat{R}}.$$  

(61)

It is useful to express the .632+ estimator in terms of its predecessor, the .632 estimator. Combining (55), (58), and (59) then substituting in (60) yields:

$$\overline{Err}_t^{(632+)} = \overline{Err}_t^{(632)} + (\overline{Err}_t^{(1)} - \overline{Err}_t) \frac{.368 \cdot .632 \cdot \hat{R}}{1 - .368 \hat{R}}.$$  

(62)

Efron and Tibshirani (1997) consider the possibility that $\hat{R}$ lies out of the region $[0, 1]$. This leads to their proposal of defining:

$$\overline{Err}_t^{(632+)} = \min(\overline{Err}_t^{(1)}, \hat{\gamma}),$$  

(63)

$$\hat{R}_t = \left\{ \begin{array}{ll} (\overline{Err}_t^{(1)} - \overline{Err}_t) / (\hat{\gamma} - \overline{Err}_t) & \overline{Err}_t < \overline{Err}_t^{(1)} < \gamma \\ 0 & \text{otherwise} \end{array} \right.$$  

(64)

to obtain a modification to (62) that becomes:

$$\overline{Err}_t^{(632+)} = \overline{Err}_t^{(632)} + (\overline{Err}_t^{(1)} - \overline{Err}_t) \frac{.368 \cdot .632 \cdot \hat{R}_t}{1 - .368 \hat{R}_t}.$$  

(65)

### 3.4. Estimating the Standard Error of Error Rate Estimators

What have been discussed above are different methods to estimate the error rate of a trained classification rule, e.g., cross validation, .632, .632+, conditional on that training set; alternatively, to estimate the mean error rate, as an expectation over the population of training datasets, like the LOOB estimator. Regardless of what the estimator is designed to estimate, it is still a function of the current dataset $t$, i.e., it is a random variable. If $\overline{Err}_t^{(1)}$ is considered, it estimates a constant real-valued parameter $E_{\theta \eta} E_{x_0} L(y_0, \eta(x_0))$ with expectation taken over all the trainers and then over all the testers, respectively; this is the overall mean error rate. Yet, $\overline{Err}_t^{(1)}$ is a random variable whose variability comes from the finite size of the available dataset. If the classifier is trained and tested on a very large number of observations, this would approximate training and testing on the entire population, and the variability would shrink to zero. This also applies for any performance measure other than the error rate.

The next question then is, having estimated the mean performance of a classifier, what is the associated uncertainty of this estimator, i.e., can an estimate of the variance of this estimator be obtained from the same training dataset? Efron and Tibshirani (1995) proposed using the influence function method, see Section 2.4, to estimate the uncertainty (variability) in $\overline{Err}_t^{(1)}$. The reader is alerted that estimators that incorporate a piece of the apparent error are not suitable for the influence function method. Such estimators are not smooth because the apparent error is not smooth. By recalling the definitions of Section 2.4, $\overline{Err}_t^{(1)}$ is now the statistic $s(\hat{F})$. Define $N^b_i$ to be the number of times the case $t_i$ is included in the bootstrap $b$. Also, define the following notation:

$$I^b_i = \frac{1}{n} \sum_{i=1}^{n} I^b_i t_i.$$  

(66)

It has been proven in Efron and Tibshirani (1995) that the influence function of such an estimator is given by:

$$\frac{\partial s(\hat{F}_{x_i})}{\partial \varepsilon} \bigg|_{\varepsilon=0} = (2 + \frac{1}{n-1}) (\hat{E}_i - \overline{Err}_t^{(1)}) + \frac{n \sum_{b=1}^{B} (N^b_i - \overline{N}_i) I^b_i}{\sum_{b=1}^{B} I^b_i}.$$  

(67)

Combining (40) and (67) gives an estimation to the uncertainty in $\overline{Err}_t^{(1)}$. 

1
4. Nonparametric Methods for Estimating the AUC of a Classification Rule

In the present section, we extend the study carried out in Efron (1983); Efron and Tibshirani (1997), and summarized in Section 3, to construct nonparametric estimators for the AUC analogue to those of the error rate. Previous experimental and comparative studies have been conducted by considering the .632 bootstrap and the LOOCV (Yousef et al., 2005; Sahinler et al., 2001, 2008) with no enough theoretical justification. We provide here a full account of the different versions of bootstrap estimators reviewed in Section 3 and show how they can be formally extended to estimate the AUC.

4.1. Construction of Nonparametric Estimators for AUC

Before switching to the AUC some more elaboration on Section 3 is needed. The SB estimator (46) can be rewritten as:

$$E_{err}^{SB} = E_x E_{F_{ci}} [L(q_{i*}(x), y)|t^*].$$

Since there would be some observation overlap between the $t$ and $t^*$ this approach suffers an obvious bias as was introduced in that section. This was the motivation behind interchanging the expectations and defining the LOOB (Section 3.3.1). Alternatively, we could have left the order of the expectation but with testing on only those observations in $t$ that do not appear in the bootstrap replication $t^*$, i.e., the distribution $\hat{F}^{(*)}$. We call the resulting estimator $E_{err}^{(*)}$, which is given formally by:

$$E_{err}^{(*)} = E_x E_{F_{ci}} [L(q_{i*}(x), y)|t^*].$$

Analogously to Section 3 and to what has been introduced above, we can define several bootstrap estimators for the AUC. The start is the SB estimate which can be written as:

$$\bar{AUC}^{SB}_t = E_x [AUC_{t^*}(\hat{F}).$$

This averages the Mann-Whitney statistic over the bootstraps, where $AUC_{t^*}(\hat{F})$ refers to the AUC obtained from training the classifier on the bootstrap replicate $t^*$ and testing it on the empirical distribution $\hat{F}$. In the approach used here, the bootstrap replicate $t^*$ preserves the ratio between $n_1$ and $n_2$. That is, the training sample $t$ is treated as $t = t_1 \cup t_2$, $t_1 \in \omega_1$ and $t_2 \in \omega_2$ then $n_1$ cases are replicated from the first-class sample and $n_2$ cases are replicated from the second-class sample to produce $t^*_1$ and $t^*_2$ respectively, where $t^* = t^*_1 \cup t^*_2$. This was not needed when the performance measure was the error rate since it is a statistic that does not operate simultaneously on two different datasets as the Mann-Whitney statistic does (in $U$-statistic theory (Randles and Wolfe, 1979), error rate and Mann-Whitney are called one-sample and two-sample statistics respectively). For a limited number of bootstraps the expectation (71) is approximated by:

$$\bar{AUC}^{SB}_t = \frac{1}{B} \sum_{b=1}^{B} [AUC_{t^b}(\hat{F})],$$

i.e., averaging over the $B$ bootstraps for the AUC obtained from training the classifier on the bootstrap replicate $t^b$ and testing it on the original dataset $t$.

The same motivation behind the estimator (49) can be applied here, i.e., testing only on those cases in $t$ that are not included in the training set $t^b$ in order to reduce the bias. This can be carried out in (74) without interchanging the summation order. The new estimator is named $\bar{AUC}^{(*)}_t$, where the parenthesis notation $(*)$ refers to the exclusion, in the testing stage, of the training cases that were generated from the bootstrap replication. Formally, this is written as:

$$\bar{AUC}^{(*)}_t = \frac{1}{B} \sum_{b=1}^{B} [AUC_{t^b}(\hat{F}^{(*)})]$$

$$= \frac{1}{B} \sum_{b=1}^{B} \left[ \sum_{j=1}^{n_2} \sum_{i=1}^{n_1} \psi(\hat{h}_{i*}(x_i), \hat{h}_{j*}(x_j)) \sum_{b=1}^{B} I^b_j \sum_{i=1}^{n_1} I^b_i \sum_{j=1}^{n_2} I^b_j \right].$$
The 0.632 estimator can be introduced here in the same way it was used for the true error rate (see Section 3.3.3). The true AUC for the classifier if trained on a particular training dataset $t$ can be written as:

$$AUC_t = AUC_t + \varepsilon_t(AUC_t^a(\hat{F}) - AUC_t^a).$$  

(77)

This is the same approach developed in Section 3.3.2 for the error rate. If testing is carried out on cases excluded from the bootstraps, then (77) can be approximated analogously to what was done in Section 3.3.3. This gives rise to the 0.632 AUC estimator:

$$AUC_t^{(632)} = 0.368 AUC_t + 0.632 AUC_t^a.$$  

(78)

It should be noted that this estimator is designed to estimate the true AUC for a classifier trained on the dataset $t$ (the classifier performance conditional on the training dataset $t$). This is on contrary to the estimator (75) that estimates the mean performance of the classifier (this is the expectation over the training set population for the conditional performance).

The 0.632+ estimator $AUC_t^{(632,+)}$ develops from $AUC_t^{(632)}$ in the same way as $\hat{Err}_t^{(632,+)}$ developed from $\hat{Err}_t^{(632)}$ in Section 3.3.4. There are two modifications to the details. The first regards the no-information error rate $\gamma$; Lemma 1 shows that the no-information AUC is given by $\gamma_{AUC} = 0.5$. The second regards the definitions (63), which should be modified to accommodate for the AUC. The new definitions are given by:

$$AUC_t^{(632,+)} = AUC_t^{(632)} + (AUC_t^a - AUC_t^*)  
\times \frac{368 \cdot \hat{R}'}{1 - 368 \hat{R}'}.$$  

(79)

$$AUC_t^* = \max(AUC_t^a, \gamma_{AUC}),$$  

(80)

$$\hat{R}' = \begin{cases} (AUC_t^a - AUC_t^*)/(\gamma_{AUC} - AUC_t^a) & \text{if } AUC_t^a > AUC_t^* > \gamma_{AUC} \\ 0 & \text{otherwise}. \end{cases}$$  

(81)

To this end, we have constructed the AUC nonparametric estimators analogue to those of the error rate. Some of them, mainly the .632+ estimator, will have the least bias as will be shown in Section 5. However, all of these estimators are not “smooth” and not eligible for the variance estimation via, e.g., the influence function approach (Sections 2.4 and 3.4). Before we desing the new estimator (Section 4.3), the smoothness issue needs more elaboration in the next section.

4.2. Smoothness of Estimators

For better understanding for the smoothness issue, consider the very simple case where there are just two features and the classifier is the LDA, where the decision surface will be a straight line in the bi-feature plane (generally, it will be a $p$-dimensional feature space). Also for simplicity and better pedagogy, consider the true error as the performance measure of interest rather than the AUC.

The $\hat{Err}_t^{(632)}$, defined in (70), is the expectation over the bootstraps for the error rate that come from training on a bootstrap replicate and testing on only those cases not included in that bootstrap training sample. The concept of the influence function (Section 2.4) can be implemented by perturbing a sample case and studying its effect on the variability of the estimator. This perturbation of course propagates through to the probability masses of the bootstrap replicates as well. It can be shown that (see Efron, 1992) the bootstrap $b$ includes the case $i$, $N_b^t$ times with probability $g_{e,i}^t$ given by

$$g_{e,i}^t(b) = (1 - \varepsilon)^n(1 + \frac{n \varepsilon}{1 - \varepsilon})^{N_b^t} (1/(n))^{N_b^t}. $$

(82)

Then, the estimator $\hat{Err}_t^{(632)}$, after perturbation, is evaluated as

$$\hat{Err}_t^{(632)}(\hat{F}_{e,i}) = \sum_b g_{e,i}^t \hat{Err}_t^{(632)}(\hat{F}_{e,i}). $$

(83)

The reader should note that if there is no perturbation, i.e., $\varepsilon$ is set to zero, (83) is merely reduced to an averaging over the bootstraps.

A simple simulation in this bi-feature problem mentioned above was carried out using 1000 bootstraps. The decision surfaces obtained from the first five bootstrap replicates are shown in Figure 4. A sample is generated from each of two classes and is represented in the figure together with the decision surface obtained by training on this sample. The decision surfaces obtained from the first five bootstrap replicates are shown in Figure 5. In brief
Linear Discriminant Surfaces from Different Bootstraps

Figure 4: Different linear decision surfaces obtained by training on different bootstrap replicates from the same training dataset. The first case from class 1 is chosen for perturbation. Changing a feature, e.g., $X_1$, has no change on the decision value of a single surface unless the case crosses that surface.

Estimated True Error vs. Perturbation in First Feature

Figure 5: The two estimators $\hat{\text{Err}}_t^{(1)}$, $\hat{\text{Err}}_t^{(*)}$, and the component $\text{Err}_t^{(*)}(\hat{F}_{\varepsilon,i}^{(1)})$ estimated after training on the first bootstrap replicate. The first two are smooth while the third is not. The estimated true error is plotted vs. change in the value of the first feature.

$\hat{\text{Err}}_t^{(*)}$ and $\hat{\text{Err}}_t^{(1)}$ almost give the same estimated value and both are smooth. However, the former has a smooth inner summation, which makes it suitable for using the differential operator of the influence function. On the contrary, the latter has a non-smooth inner summation, which is not suitable for the differential operator of the influence function.

It is worth mentioning that similar argument follows to show how cross validation estimator is not smooth. Consider the decision surface in the feature subspace that results from training the classifier on the dataset that remains after leaving out the case $t_i$. Whenever the predictor $x_i$ changes, the loss function will not change unless the predictor passes across the decision surface. To recap, training on many datasets results in many decision surfaces and then whenever the predictor $x_i$ changes it will tend to cross some of the surfaces, yielding a smoother estimator, rather than the discontinuous one that results from CV or any other similar estimator.

4.3. The Leave-Pair-Out Bootstrap (LPOB) $\hat{\text{AUC}}_t^{(1,1)}$, Its Smoothness, and Variance Estimation

Now turning back to the AUC, the only estimator constructed in Section 4.1 that may seem smooth, and hence may be suitable for applying the influence function method of variance estimation is the $\hat{\text{AUC}}_t^{(*)}$. However, Yousef et al. (2005) proved that the analogue to (82)–(83) are:

$$g_{k_{\varepsilon,i}}(b) = (1-\varepsilon)^{n_k} (1 + \frac{n_k \varepsilon}{1-\varepsilon})^{N_b} (1/n_1)^{n_1} (1/n_2)^{n_2},$$

$$\hat{\text{AUC}}_t^{(*)}(\hat{F}_{\varepsilon,i}^{(1)}) = \sum_b g_{\varepsilon,i}^{(1)} \hat{\text{AUC}}_t^{(*)}(\hat{F}_{\varepsilon,i}^{(1)}).$$

Same argument made above (in Section 4.2) for $\text{Err}_t^{(*)}$ is immediate here for $\hat{\text{AUC}}_t^{(*)}$. Applying the influence function to the $\hat{\text{AUC}}_t^{(*)}$ statistic enforces distributing the differential operator $\partial/\partial \varepsilon$ over the summation to be encountered by the unsmooth statistic $\hat{\text{AUC}}_t^{(*)}(\hat{F}_{\varepsilon,i}^{(1)})$ in (85). It is unsmooth since the classifier is trained on just one dataset.

The above discussion suggests introducing an analogue to $\hat{\text{Err}}_t^{(1)}$ for measuring the performance in AUC. This estimator
is motivated from (71) the same way the estimator $\widehat{Err}_1^{(1)}$ was motivated from (48). The SB estimator (71) can be rewritten as:

$$\widehat{AUC}_{i,j}^{SB} = \frac{1}{n_1n_2} \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} E_x\{ \psi(\hat{h}_{i*}(x_i), \hat{h}_{i*}(x_j)) \}$$

$$\quad = \frac{1}{n_1n_2} \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \sum_{b=1}^{B} \left[ \psi(\hat{h}_{i*}(x_i), \hat{h}_{i*}(x_j))/B \right]$$

(86)

(87)

In words, the procedure is to select a pair (one observation from each class) and calculate for that pair the mean-over-two estimators. That the new AUC estimators designed in Section 4 exhibit the same behavior but with magnified difference between the estimators in terms of the experimental RMS defined by Efron as:

$$\text{MSE} = \frac{1}{G} \sum_{g=1}^{G} \left( \text{Err}_{t_g} - \text{Err}_{t_0} \right)^2$$

(89a)

(89b)

where $\text{Err}_{t_g}$ is the estimator (any estimator) conditional on a training dataset $t_g$, and $\text{Err}_{t_0}$ is the true prediction error conditional on the same training dataset. The number of MC trials, $G$, in his experiments was 200. The following statement is quoted from Efron and Tibshirani (1997): “The results vary considerably from experiment to experiment, but in terms of RMS error the .632+ rule is an overall winner.”

This conclusion was without stating the criterion for deciding the overall winner. It was apparent from their results that the .632+ rule is the winner in terms of the bias—as was designed for. We calculated the average of the RMS of every estimator across all the 24 experiments they ran; Table 1 displays these averages. The estimators $\text{Err}_{t_1}^{(1)}$ and $\text{Err}_{t_1}^{(324)}$ are quite comparable to each other with only 2.5% increase in the average RMS of the former. We will show below in Section 5.2 that the new AUC estimators designed in Section 4 exhibit the same behavior but with magnified difference between the two estimators.

5. Experimental Results

5.1. Error Rate Estimation

Efron (1983); Efron and Tibshirani (1997) provide comparisons of their proposed estimators (discussed in Section 3) including estimating the standard error of the smooth LOOB estimator $\widehat{Err}_1^{(1)}$ using the influence function approach. They ran many simulations considering a variety of classifiers and data distributions, as well as real datasets. They assessed the estimators in terms of the experimental RMS defined by Efron as:

5.2. AUC Estimation

We carried out different experiments to compare the three bootstrap-based estimators $\widehat{AUC}_{i}^{(1)}$, $\widehat{AUC}_{i}^{(632)}$, and $\widehat{AUC}_{i}^{(632+)}$ of Section 4, considering different dimensionalities, different parameter values, and training set sizes. All experiments provided consistent and similar results. Here in this section we illustrate the results when the dimensionality $p = 5$ for multivariate data with $\Sigma_1 = \Sigma_2 = I$, $\mu_1 = 0$, $\mu_2 = cI$, and $c$ is an adjusting parameter to adjust the Mahalanobis distance $D = [(\mu_1 - \mu_2)\Sigma^{-1}(\mu_1 - \mu_2)]^{1/2} = c^2 p$. We adjust $c$ to keep a reasonable inter-class separation of $\Delta = 0.8$. When the classifier
is trained, it will be tested on a pseudo-infinite test set, here 1000 cases per class, to obtain a very good approximation to the true AUC for the classifier trained on this very training data set; this is called a single realization or a Monte-Carlo (MC) trial. Many realizations of the training data sets with same $n$ are generated over MC simulation to study the mean and variance of the AUC for the Bayes classifier under this training set size. The number of MC trials is 1000 and the number of bootstraps is 100. It is apparent from Figure 6 that the $\hat{AUC}_t$ is downward biased. This is a natural opposite of the upward bias observed in Efron and Tibshirani (1997) when the performance measure was the true error rate as a measure of incorrectness, by contrast with the true AUC as a measure of correctness. The $\hat{AUC}_t$ is designed as a correction for $\hat{AUC}_t$; it appears in the figure to correct for that but with an over-shoot. The correct adjustment for the remaining bias is almost achieved by the estimator $\hat{AUC}_t(632)$. The $\hat{AUC}_t(632)$ estimator can be seen as an attempt to balance between the two extreme biased estimators, $\hat{AUC}_t$ and $\hat{AUC}_t$. However, it is expected that the component of $\hat{AUC}_t$ that is inherent in both $\hat{AUC}_t(632)$ and $\hat{AUC}_t(632)$ increases the variance of these two estimators that my compensate for the decrease in the bias. Therefore, we assess all estimators in terms of the RMS, as defined in (89). Table 2 gives a comparison for these different estimators in terms of the RMS. We average the RMS of these estimators over the 10 experiments of Table 2 and list the average in Table 3. It is evident that the .632+ is slightly the overall winner with only 9% decrease in RMS if compared to the $\hat{AUC}_t$ estimator. This almost agrees with the same result obtained for the error rate estimators and reported in Table 1.

In addition to the RMS, Table 2 compares the estimators in terms of the RMS around the mean, i.e., the mean over all possible training sets, instead of the conditional performance on a particular training set. The motivation behind that is explained next. The estimators $\hat{AUC}_t$ and $\hat{AUC}_t(1.1)$ seem, at least from their formalization, to estimate the mean AUC of the classifier (this is the analogue of $\hat{\Delta}_t$ and $\hat{\Delta}_t(1.1)$). However, the basic motivation for the $\hat{AUC}_t(632)$ and $\hat{AUC}_t(632+)$ is to estimate the AUC conditional on the given dataset $t$ (this is the analogue of $\hat{\Delta}_t(632)$ and $\hat{\Delta}_t(632+)$). Nevertheless, as mentioned in Efron and Tibshirani (1997) and detailed in Zhang (1995) the CV, the basic ingredient of the bootstrap based estimators, is weakly correlated with the true performance on a sample by sample basis. This means that no estimator has a preference in estimating the conditional performance (Remark 1, Section 5.4).

5.3. Two Competing Classifiers

If the assessment problem is how to compare two classifiers, rather than the individual performance, then the measure to be used is either the conditional difference

$$\Delta_t = AUC_{1t} - AUC_{2t},$$

(90)
or the mean, unconditional, difference
\[ \Delta = \mathbb{E}[AUC_1 - AUC_2], \]
where, we defined them for the AUC just for illustration with immediate identical treatment for other measures. Then it is obvious that there is nothing new in the estimation task, i.e., it is merely the difference of the performance estimate of each classifier, i.e.,
\[ \tilde{\Delta} = \mathbb{E}[AUC_{1*} - AUC_{2*}], \]
where each of the two estimators in (92) is obtained by any of the estimators discussed in Section 3 for error rate or Section 4 for the AUC. A natural candidate, from the point of view of the present article is the LPOB estimator \( \hat{AUC}_{(1,1)} \) —because of both the smoothness and weak correlation issues discussed in Sections 4.2 and 5.2 respectively.

Then, how to estimate the uncertainty (variance) of \( \tilde{\Delta} \). This is very similar to estimating the variance in \( \mathbb{E}[\hat{AUC}_t] \), mentioned in section 4.4 and detailed in Yousef et al. (2005). There is nothing new in estimating \( \text{Var}\tilde{\Delta} \). It is obtained by replacing \( \hat{AUC}_{(1,1)} \), in Yousef et al. (2005), by the statistic \( \tilde{\Delta} \) in (92). For demonstration, typical values are given in Table 4, for comparing the linear and quadratic discriminants, where the training set size per class is 20 and number of features is 4. A final remark for uncertainty estimation is provided in Remark 2, Section 5.4.

5.4. Final Remarks

Remark 1 (conditional vs. mean performance). We note that there are several points of view regarding the relative utility of measuring the “true performance”, i.e., the performance conditional on a given training dataset, versus estimating the mean performance over the population of training sets. Some users might argue that the conditional performance is the most appropriate, claiming that they will freeze the trainers. However, this does not really correspond to the practical world in which practitioners up-date the training as more data becomes available; in that case the target would be the expected performance over the population of trainers. Nevertheless, and unfortunately, this idealistic argument is refuted by the empirical results of the weak correlation between the estimators and the conditional performance (Section 5.2).

Remark 2 (estimating the uncertainty of performance estimators). Estimating the uncertainty in the estimator of \( \text{Err}, \text{AUC} \), or the difference performance \( \Delta \), should in fact be a central point for the field of machine learning. Most practitioners simply provide simple estimates of the conditional performance of their favorite classifier, and similarly for a competing classifier. It is rare to see estimates of the uncertainty of measures of classifier performance, and especially rare to see estimates of the uncertainty in the difference of measures of performance of competing classifiers.

Remark 3 (support size of bootstrap). As shown by Efron and Tibshirani (1997), the \( \hat{E}_{*}\) estimator is a smoothed version of the LOOCV, since for every test sample case the classifier is trained on many bootstrap replicates. This reduces the variability of the CV based estimator. On the other hand, the effective number of cases included in the bootstrap replicates is .632 of the total sample size \( n \). This accounts for training on a less effective dataset size; this makes the LOOB estimator \( \hat{E}_{(1)} \) more biased than the LOOCV. This bias issue is observed as well when the performance measure was the AUC Sahiner et al. (2001); Yousef et al. (2005); Sahiner et al. (2008). This fact is illustrated in Figure 7 for \( \hat{AUC}_{(*)} \). At every sample size \( n \) the true value of the AUC is plotted. The estimated value \( \hat{AUC}_{(*)} \) at data sizes of \( n/.632 \) and \( n/.5 \) are plotted as well. It is obvious that these values are lower and higher than the true value respectively, which supports the discussion of whether the LOOB is supported on 0.632 of the cases or 0.5 of the cases (as mentioned in Efron and Tibshirani (1997)) or, as here, something in-between. It is worth mentioning that if the resampling mechanism only cares about the observations appeared in the bootstrap replication without caring about their order, i.e., sampling is with replacement without ordering, the bootstrap will be supported on almost 0.5 as opposed to 0.632 (Lemma 2 in Appendix).
6. Conclusion

This article started with reviewing the nonparametric estimators that estimate the mean and variance of any one-sample statistic, in general, and the error rate of a classification rule, in particular. Then, we extended these estimators from estimating the error rate (a one-sample statistic) to estimating the AUC (a two-sample statistic). This extension is theoretically justified and not just an ad-hoc application. This extension is supported by a set of experiments to illustrate their relative accuracy in terms of the RMS. Among those estimators, we identified those that are smooth and eligible for the variance estimation using the influence function approach. In addition, we provided experimental examples to illustrate the smoothness issue that is mentioned tersely in many articles in literature. The set of experiments supports that the performance of our AUC estimators complies with that of the error rate estimator in the following: all bootstrap versions have almost the same accuracy, measured in terms of RMS, with little superiority of the .632+ bootstrap estimator; and all estimators have a weak correlation with the conditional AUC exactly as the error rate estimators are weakly correlated with the conditional error rate.

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8. Appendix

**Lemma 1.** The no-information AUC is given by $\gamma_{AUC} = 0.5$.

**Proof.** The no-information $AUC, \gamma_{AUC}$, an analogue to the no-information error rate, $\gamma$, is given by (3) but with TPF and FPF given under the no-information distribution $E_{0\mathcal{F}}$ (see Section 3.3.4). Therefore, assume that there are $n_1$ cases from class $\omega_1$ and $n_2$ cases from class $\omega_2$. Assume also for fixed threshold $th$ the two quantities that define the error rate for this threshold value are TPF and FPF. Also, assume that the sample cases are tested by the classifier and each sample has been assigned a decision value (score). Under the no-information distribution, consider the following. For every decision value $h_i(x_i)$ assigned for the case $i = (x_i, y_i)$, create new $n_1 + n_2 - 1$ cases; all of them have the same decision value $h_i(x_i)$, while their responses are equal to the responses of the rest $n_1 + n_2 - 1$ cases $j$, $j \neq i$. Under this new sample that consists of $(n_1 + n_2)^2$ cases, it is quite easy to see that the new TPF and FPF for the same threshold $th$ are given by:

$$FPF_{\hat{x}_i,th} = TPF_{\hat{x}_i,th} = \frac{TPF \cdot n_1 + FPF \cdot n_2}{(n_1 + n_2)}.$$

This means that the ROC curve under the no-information rate is a straight line with slope equal to one; this directly gives $\gamma_{AUC} = 0.5$.

**Lemma 2 (0.632- or 0.5-bootstrap?).** The bootstrap is supported on half of the observations, i.e., on average half of the observations appear in a bootstrap replication, if we consider sampling with replacement without ordering.

**Proof.** That an observation does not appear in a bootstrap is equivalent to sampling with replacement and without ordering the $n$ observations from all $n$ observations except that one. Then the probability to appear in this bootstrap is

$$1 - Pr\left[\hat{x}_i^b = 1\right] = 1 - \frac{(n-1) + n - 1}{n} \left(\frac{2n-1}{n}\right) = \frac{n}{2(2n-1)} \cong 1/2. \quad (93)$$

This result is trivial because it can be read off the normalized binomial distribution for $n$ trials with probability $1/2$.

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Efron, B., 1992. Jackknife-After-Bootstrap Standard Errors and Influence Functions. Journal of the Royal Statistical Society. Series B (Methodological) 54, 83–127.
| Estimator | Mean  | SD    | RMS   | RMS around mean | Corr. Coef. | Size |
|-----------|-------|-------|-------|-----------------|-------------|------|
| $AUC_t^1$ | 0.6181| 0.0434| 0     | 0.0434          | 1.0000      | 1.0  |
| $AUC_t^1$ | 0.5914| 0.0947| 0.0973| 0.0984          | 0.2553      |      |
| $AUC_t^1$ | 0.7012| 0.0749| 0.1128| 0.1119          | 0.2559      | 20   |
| $AUC_t^1$ | 0.6431| 0.0858| 0.0906| 0.0894          | 0.2218      |      |
| $AUC_t^1$ | 0.8897| 0.0475| 0.2774| 0.2757          | 0.2231      |      |
| $AUC_t^1$ | 0.6231| 0.0410| 0     | 0.0410          | 1.0000      | 1.0  |
| $AUC_t^1$ | 0.5945| 0.0947| 0.0973| 0.0984          | 0.2553      |      |
| $AUC_t^1$ | 0.7012| 0.0749| 0.1128| 0.1119          | 0.2559      | 20   |
| $AUC_t^1$ | 0.6431| 0.0858| 0.0906| 0.0894          | 0.2218      |      |
| $AUC_t^1$ | 0.8897| 0.0475| 0.2774| 0.2757          | 0.2231      |      |
| $AUC_t^1$ | 0.6308| 0.0400| 0     | 0.0400          | 1.0000      | 1.0  |
| $AUC_t^1$ | 0.5991| 0.0947| 0.0973| 0.0984          | 0.2553      |      |
| $AUC_t^1$ | 0.7012| 0.0749| 0.1128| 0.1119          | 0.2559      | 20   |
| $AUC_t^1$ | 0.6431| 0.0858| 0.0906| 0.0894          | 0.2218      |      |
| $AUC_t^1$ | 0.8897| 0.0475| 0.2774| 0.2757          | 0.2231      |      |

Table 2: Comparison of the different bootstrap-based estimators of the $AUC_t$; they are comparable to each other in the RMS sense, $AUC_t^1$ is almost unbiased, and all are weakly correlated with the true conditional performance $AUC_t$.
Table 3: Average of RMS error of each estimator over the 10 experiments displayed in Table 2. The estimator $\overline{AUC}_t^{(*)}$ is the next to $\overline{AUC}_t^{0.632+}$ with only 9% increase in RMS.

| Estimator     | Average RMS |
|---------------|-------------|
| $AUC_t$       | 0           |
| $\overline{AUC}_t^{(*)}$ | .07347     |
| $AUC_t^{0.632}$ | .07409     |
| $\overline{AUC}_t^{0.632+}$ | .06735     |
| $\overline{AUC}_t$ | .17808     |

Table 4: Estimating the uncertainty in the estimator that estimates the difference in performance of two competing classifiers, the LDA and the QDA. The quantity $M$ represents $AUC_1$ for LDA, $AUC_2$ for QDA, and $\Delta$ for the difference.

| Metric $M$ | LDA | QDA | Diff. |
|------------|-----|-----|-------|
| E $M_t$   | .7706 | .7163 | .0543 |
| SD $M_t$  | .0313 | .0442 | .0343 |
| E $\widehat{M}^{(1,1)}$ | .7437 | .6679 | .0758 |
| SD $\widehat{M}^{(1,1)}$ | .0879 | .0944 | .0533 |
| E SD $\widehat{M}^{(1,1)}$ | .0898 | .1003 | .0708 |
| SD SD $\widehat{M}^{(1,1)}$ | .0192 | .0163 | .0228 |