A Leisurely Look at Versions and Variants of the Cross Validation Estimator

Waleed A. Yousef

Ph.D., Computer Science Department, Faculty of Computers and Information, Helwan University, Egypt.
Human Computer Interaction Laboratory (HCI Lab.), Egypt.

Abstract
Many versions of cross-validation (CV) exist in the literature; and each version though has different variants. All are used interchangeably by many practitioners; yet, without explanation to the connection or difference among them. This article has three contributions. First, it starts by mathematical formalization of these different versions and variants that estimate the error rate and the Area Under the ROC Curve (AUC) of a classification rule, to show the connection and difference among them. Second, we prove some of their properties and prove that many variants are either redundant or "not smooth". Hence, we suggest to abandon all redundant versions and variants and only keep the leave-one-out, the K-fold, and the repeated K-fold. We show that the latter is the only among the three versions that is "smooth" and hence looks mathematically like estimating the mean performance of the classification rules. However, empirically, for the known phenomenon of "weak correlation", which we explain mathematically and experimentally, it estimates both conditional and mean performance almost with the same accuracy. Third, we conclude the article with suggesting two research points that may answer the remaining question of whether we can come up with a finalist among the three estimators: (1) a comparative study, that is much more comprehensive than those available in literature and conclude no overall winner, is needed to consider a wide range of distributions, datasets, and classifiers including complex ones obtained via the recent deep learning approach. (2) we sketch the path of deriving a rigorous method for estimating the variance of the only "smooth" version, repeated K-fold CV, rather than those ad-hoc methods available in the literature that ignore the covariance structure among the folds of CV.

Keywords: Cross-Validation, CV, Bootstrap, Error, Receiver Operating Characteristics, ROC, Area Under the Curve, AUC, Influence Function.

1. Introduction

1.1. Background and Motivation
The early motivation behind our present article started since our contribution in the MAQC project, which was formally launched by scientists at the FDA's National Center for Toxicological Research (NCTR), Jefferson, Arkansas, in response to the FDA Critical Path Initiative. MAQC was a group of over 100 members from industry, academia, and US government working on methods for developing predictive models that use high-dimensional microarray (DNA chips) data to classify patients into low- or high-risk with respect to getting a specified kind of cancer. In particular, phase II of the MAQC project (MAQCII) aimed at providing the best practices to design DNA microarray classification methods. This is, in many cases, an ill-posed problem since the dimensionality (number of genes) is in thousands whereas the number of observations (patients) is in hundreds. Classifiers designed for such a problem can easily suffer from large variability (unstability); hence they may not generalize, and results obtained from the studies are fragile. Our main conclusion of the project was published in Nature biotechnology (Shi et al., 2010), in addition to other several publications each was an in-depth treatment of a technical aspect of the project.

One of these publications is Chen et al. (2012b), in which we discussed the uncertainty (standard error) estimation associated with the assessment of classification models under the scarcity of data, where we applied the techniques developed earlier in Yousef et al. (2005, 2006) to assess classifiers in two different paradigms. In Paradigm I (Yousef et al., 2005), the classifier is assessed from only one available dataset, where resampling must take place to train and test on two different datasets in each resampling iteration. However, the resampling approach is a "smooth" version of the bootstrap (BS) rather than the Cross Validation (CV); therefore, the variance of the former can be estimated almost unbiasedly using the Influence Function (IF) approach derived in (Efron and Tibshirani, 1997) for the error rate and extended in Yousef et al. (2005) for the AUC. This is as opposed to the CV estimators where only ad-hoc estimators of their standard error are available that ignore the covariance structure among folds, and no unbiased estimator of their variance exists (Bengio and Grandvalet, 2004). In paradigm II (Yousef et al., 2006), elaborated later in Chen et al. (2012a), it is assumed that the assessment must be carried over two independent and sequestered datasets, one for training and one for testing. This protocol is
mandatory in some regulatory agencies, e.g., the FDA. In this paradigm, the performance estimate for either the error rate or the AUC, along with their variance estimation, are obtained via the Uniform Minimum Variance Unbiased Estimator (UMVUE) derived from the $U$-statistic theory (Randles and Wolfe, 1979).

Part of the scientific debate, in particular among colleagues of the project that time, or in general in the whole field, is on the assessment strategy and the several versions of estimators that practitioners do (or should) use under paradigm I, and which estimator is “better” and in which “sense”? Although the BS based estimators are “smooth” and their standard error can be estimated using the IF method as just mentioned, many, including some giants and fathers of the field, prefer the CV estimators for their simplicity and “they are easier to explain” (personal communication with Robert Tibshirani, Washington, DC., circa 2004, who is himself a coauthor of (Efron and Tibshirani, 1997) that adopts the BS and IF approaches).

The debate becomes louder when adopting CV, for that many versions exist in the literature that are used loosely without understanding the connection or difference among them. To name a few: leave-one-out CV, $K$-fold CV, repeated CV, and Monte-Carlo CV; e.g., see Kuhn and Johnson (2013); Dubitzky et al. (2007); Xu and Liang (2001); Arlot et al. (2010); Shi et al. (2010). Each of these versions has some variants (e.g., whether to first sum over folds or over observations), which may be thought of as trivially equal. However, as will be shown in Section 2 they are not. Therefore, two legitimate themes of questions arise, and outlined below.

First, we need to understand what connection or difference is among those versions or variants. Do they have same properties? Do they have different properties when estimating the AUC of a classification rule rather than its error rate? Can we show that some of them are trivial (or identical) variations of others, drop them out, and hence filter the literature? Are they designed, at least theoretically, to estimate the mean or conditional performance of classification rules? These questions are answered in the present article. We conclude the article with suggesting a computational and comprehensive comparative study that should consider several distributions, datasets, classifiers, and deep learning architectures, to compare among the final filtered versions. Such a study will be complementary to the present article and may contribute to the best practices than the current wisdom that says no overall winner among them.

Second, can we find an estimator of the variance of any of these versions as opposed to the ad-hoc methods used in the literature that almost use the sample variance procedure among folds? This is out of scope of the present article and is a stand alone research that we propose in Section 5 and sketch out one possible direction for it.

1.2. Notation

We treat the binary classification problem where a classification rule is trained on the training set $X$ and provide a score $h_X(x)$ when tested on an observation $x$, which will be classified as either belonging to class 1 (or class 2) based on whether $h_X(x)$ is less (or larger) than a chosen threshold value $t_h$. Two important performance measures used to assess the classification rules are the error rate and the Area Under the ROC Curve (AUC).

In this article, we analyze the CV estimators used for assessing classifiers in terms of these two measures. For the error rate, we use the notation $Q(x,X)$, where $Q$ is the zero-one loss function to denote miss (or correct) classification of observation $x$. For the AUC, we use the notation

$$\overline{AUC} = \frac{1}{n_1 n_2} \sum_i \sum_j \psi(h_X(x_i), h_X(y_j)),$$

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

which means a classifier trained on the training set $X$ is tested on the two observations $x_i$ and $y_j$, from class 1 and class 2 respectively, to produce a single value using the kernel $\psi$, which is the kernel of the Mann-Whitney statistic, two-sample statistic of rank tests (Randles and Wolfe, 1979; Hājek et al., 1999); and then averaged over the $n_1 \times n_2$ observations of the testing set. In this notation, we preserve $y_j$ to denote an observation from class 2 and $x_i$ to denote an observation from class 1.

1.3. Manuscript Roadmap

The rest of this article is organized as follows. Section 2 provides the mathematical formalization and analysis for the main versions and variants of the CV-based estimators, as they appear in literature. In every subsection we analyze one of the versions: leave-one-out CV, $K$-fold CV, repeated CV, and Monte-Carlo CV. For each version, we consider its different variants and promote only one of them to reach the finalists in the following section. Although the paper concerns the different versions of cross validation, the leave-one-out bootstrap estimator is included in this comparison for the close connection to the cross validation, to see one unified blueprint. We tried to keep the section as lucid as possible by deferring all proofs to the Appendix. Section 3 is a theoretical critique, based on the analysis of the preceding section, to understand the theoretical difference among the versions of CV (a variant from each version). It discusses as well the important issue of whether these estimators estimate conditional performance or the mean performance. Section 4 illustrates experimentally the weak correlation issue of the CV estimators and how it is almost impossible to estimate the conditional performance using such estimators. Section 5 concludes the article, discusses its findings for a clearer vision for practitioners, and
suggests the future research to complement this article and to hopefully close the loop regarding the practical utility of having different versions of CV-based estimators.

2. Mathematical Formalization of Different Versions of the Cross Validation Estimator

2.1. Leave-One-Out Cross Validation (LOOCV)

2.1.1. Error rate

For Leave-One-Out Cross Validation estimator (LOOCV), the observation \( x_i \) is excluded and the classifier is trained on the remaining dataset \( X_{(i)} = \{ x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n \} \) (or, for short, \( X_{(i)} = \{ x_{i'} : i' \neq i \} \)), then tested on \( x_i \). The procedure is repeated \( \forall i \) and the average over all observations is calculated. Therefore, CVN for the error rate is formally defined as

\[
\overline{Err}^{(CVN)} = \frac{1}{n} \sum_{i=1}^{n} Q \left( x_i, X_{(i)} \right). \tag{3}
\]

The LOOCV is a special case of the \( K \)-fold Cross Validation (CVK) of the next section, where the former can be seen as partitioning the dataset of size \( n \) to \( N \) folds, each containing just one observation. Hence, as opposed to some literature where it is called CVN, we denote it CVN for preserving consistent notation.

2.1.2. AUC

Since AUC is a two-sample statistic, stratification is assumed for resampling. Therefore, the two datasets are sampled independently; one observation is left out from each class to produce the two sets: \( X_{(i)} = \{ x_{i'} : i' \neq i \}, X_{(j)} = \{ y_{ij'} : j' \neq j \} \). This is as opposed to treating both classes as one pool of size \( n = n_1 + n_2 \) and sampling from this common pool. Therefore, it is prudent to call the AUC CVN estimator a leave-pair-out, as we coined in Yousef et al. (2004, 2005). The classifier is trained on the set \( X_{(i)} \cup X_{(j)} \) (further, the \( \cup \) operator will be dropped for short) then tested on the two left out observations \( x_i \) and \( y_j \) to produce corresponding two scores, from which the Mannwhitney statistic (1) is calculated. The procedure is repeated \( \forall i \forall j \) and the average over all possible pairs is calculated. Therefore, the CVN for AUC is formally defined as

\[
\overline{AUC}^{(CVN)} = \frac{1}{n_1 n_2} \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \psi \left( h(x_i), h(y_j) \right), \quad h = h_{X_{(i)}X_{(j)}}. \tag{4}
\]

2.2. Conventional (one run) \( K \)-fold CV (CVK)

2.2.1. Error rate

The conventional \( K \)-fold cross validation is carried out by partitioning the dataset into \( K \) partitions (folds), training on \( K-1 \) of them and testing on the remaining one. The partitions are defined formally as follows. Define \( K: \{1, \ldots, n\} \rightarrow \{1, \ldots, K\} \), \( K = n/n_K \), such that

\[
K(i) = k, \quad n_K(k-1) < i \leq n_Kk, \quad k = 1, \ldots, K, \tag{5}
\]

and therefore, \( \sum_i 1_{(K(i)=k)} = n_K \forall k \); where for simplifying notation, and without loss of generality, \( n_K \) is assumed to be integer value. Then, the \( k^{th} \) excluded partition is \( \{ x_i : K(i) = k \} \) and the remaining dataset is \( X_{(k)} = \{ x_i : K(i) \neq k \} \). The CVN is, therefore, a special case of the CVK, where: \( K = 1, \quad K = n, \quad K(i) = i \), \( X_{(i)} = \{ x_i : K(i') \neq i \} = \{ x_i : i' \neq i \} = X_{(i)} \) (as in Section 2.1). The classifier is trained on \( X_{(k)} \) and tested on the \( k^{th} \) partition. The procedure is repeated \( V k \) and the average is calculated, once, over all tested observations. Therefore, the CVK estimator for the error rate is formally defined as

\[
\overline{Err}^{(CVK)} = \frac{1}{n} \sum_{i=1}^{n} Q \left( x_i, X_{[K(i)]} \right). \tag{6}
\]

The CVK could have been defined differently, denoted by the "stared" variant CVK*, which is easily shown to equal to the original one above:

\[
\overline{Err}^{(CVK*)} = \frac{1}{K} \sum_{k} \left[ \frac{1}{n_K} \sum_{i \in K^{-1}(k)} Q \left( x_i, X_{[k]} \right) \right]. \tag{7a}
\]

\[
= \frac{1}{Kn_K} \sum_{k} \sum_{i \in K^{-1}(k)} Q \left( x_i, X_{[k]} \right) \tag{7b}
\]

\[
= \frac{1}{n} \sum_{i} Q \left( x_i, X_{(i)} \right) \tag{7c}
\]

\[
= \overline{Err}^{(CVK)}, \tag{7d}
\]

where, in the last step, \( \sum_k \sum_{i \in K^{-1}(k)} \) and \( X_{[k]} \) are replaced by \( \sum_i \) and \( X_{(i)} \) respectively. The two variants, (6) and (7a) are equivalent. The former is the "pooled" variant, where the average is taken once over all observations. The latter is the
partitioned variant, where the average is taken individually over each partition then another average over all partitions. Although the two variants are equal, this is not the case for other estimators, e.g., the Monte-Carlo CV (Section 2.4) and the Bootstrap (Section 2.5). In addition, the partitioned variant (CVK*) can be used for estimating the variance, which is another subject that is out of scope of the present article (Section 5).

2.2.2. AUC

For the sake of generality, we assume that the number of observations \(n_1\) and \(n_2\) and, as well, the number of partitions \(K_1\) and \(K_2\) are not necessarily equal. There is no strong practical reason behind considering the general case \(K_1 \neq K_2\), except that this allows the CVN to follow naturally from the CVK as a special case by setting \(K_1 = n_1\) and \(K_2 = n_2\). Then, we have \(\mathcal{X}_k : \{1, \ldots, n_1\} \rightarrow \{1, \ldots, K_1\}\), \(K_1 = n_1/\psi_{\mathcal{K}_1}\), such that \(\mathcal{X}_k(i) = k, k = 1, \ldots, K_1,\) and \(\sum_{i=1}^{n_1} I(\mathcal{X}_k(i) = k) = n_1 K \forall k\). Similarly, the other partitioning function \(\mathcal{X}_k\) is defined. More compactly, we could have written the two partitions in one definition using a subscript \(c = 1, 2\) for the two classes respectively, as: \(\mathcal{X}_c : \{1, \ldots, n_c\} \rightarrow \{1, \ldots, K_c\}\), \(K_c = n_c/n_{cK}\), such that \(\mathcal{X}_c(i) = k_c, k_c = 1, \ldots, K_c\), and \(\sum_{i=1}^{n_c} I(\mathcal{X}_c(i) = k) = n_{cK} \forall k, c = 1, 2\).

The classifier is trained on all partitions except a partition from each class; i.e. the training set is \(\mathbf{X}_1([k_1])\) \(\mathbf{X}_2([k_2])\). Then tested on the two left-out partitions to produce corresponding two sets of \(n_1 K\) and \(n_2 K\) scores, from which \(n_1 K \times n_2 K\) pairs of Mann-Whitney statistic \(1\) are calculated. The procedure is repeated \(\forall k_1 \not\subseteq k_2\), i.e., \(K_1 \times K_2\) times, and the average Mann Whitney is calculated once over the \(n_1 \times n_2\) pooled pairs. Therefore, the CVK estimator for the AUC is given by

\[
AUC^{(CVK)} = \frac{1}{n_1 n_2} \sum_{j=1}^{n_2} \sum_{i=1}^{n_1} \psi(h(x_i), h(y_j)), \quad h = h_{\mathbf{X}_1([k_1])\mathbf{X}_2([k_2])}.
\]

Exactly as was done for the error rate above, the CVK of the AUC could have been defined in a partitioned variant (CVK*), which is easily shown to be equal to the pooled one:

\[
AUC^{(CVK*)} = \frac{1}{K_1 K_2} \sum_{k_1=1}^{K_1} \sum_{k_2=1}^{K_2} \left[ \frac{1}{n_1 K n_2 K} \sum_{i \in \mathcal{X}_1^{-1}(k_1)} \sum_{j \in \mathcal{X}_2^{-1}(k_2)} \psi(h(x_i), h(y_j)) \right], \quad h = h_{\mathbf{X}_1([k_1])\mathbf{X}_2([k_2])} \tag{9a}
\]

\[
= \frac{1}{K_1 K_2 n_1 K n_2 K} \sum_{k_1}^{n_1} \sum_{k_2}^{n_2} \sum_{i}^{n_1} \sum_{j}^{n_2} \psi(h(x_i), h(y_j)), \quad h = h_{\mathbf{X}_1([k_1])\mathbf{X}_2([k_2])} \tag{9b}
\]

\[
= \frac{1}{n_1 n_2} \sum_{j=1}^{n_2} \sum_{i=1}^{n_1} \psi(h(x_i), h(y_j)), \quad h = h_{\mathbf{X}_1([k_1])\mathbf{X}_2([k_2])} \tag{9c}
\]

\[
= AUC^{(CVK)} \tag{9d}
\]

where \(\sum_{k_1} \sum_{i \in \mathcal{X}_1^{-1}(k_1)} \sum_{k_2} \sum_{j \in \mathcal{X}_2^{-1}(k_2)} \mathbf{X}_1([k_1])\) and \(\mathbf{X}_2([k_2])\) are replaced by \(\sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \mathbf{X}_1([k_1])\) and \(\mathbf{X}_2([k_2])\) respectively. The same comment made above on the variants (6) and (7a) is literally due here on the variants (8) and (9a).

For the AUC CVK estimator, a third variant exists that we observed from experience and personal communication with some practitioners. This variant is tempting for its reduced computational speed. It is exactly the same as the partitioned variant (CVK*) but with enforcing the two left-out partitions to have the same index. This means that the classifier will be trained (and tested) only \(K\) times, rather than \(K^2\) times, each time on the two partitions \(k_1 = k_2 = k = 1, \ldots, K\). The definition of this tempting computationally reduced estimator is:

\[
AUC^{(CVK* \text{reduced})} = \frac{1}{K} \sum_{k=1}^{K} \left[ \frac{1}{n_1 K n_2 K} \sum_{i \in \mathcal{X}_1^{-1}(k)} \sum_{j \in \mathcal{X}_2^{-1}(k)} \psi(h(x_i), h(y_j)) \right], \quad h = h_{\mathbf{X}_1([k]\mathbf{X}_2([k]))} \tag{10}
\]

This computationally reduced variant is obviously not equal to the full variant (9a). Moreover, and most importantly, it exhibits more variance than the variant (9a). This rises from the fact that AUC is a two sample \(U\)-statistic (Randles and Wolfe, 1979), and to minimize its variance it is necessary to evaluate it on the total number of permutations from the two sets of observations, i.e., \(n_1 \times n_2\) times. This is guaranteed by the variant (9a). However, for the reduced variant (10) the AUC kernel will be evaluated \(K (n_1 K \times n_2 K)\) times, which will not utilize the whole number of \(n_1 \times n_2\) permutations. Clearly, this concern is not raised when formalizing the CVK estimator for the error rate since it is a one-sample statistic.

2.3. Repeated (Randomized) K-fold CV (CVKR)

2.3.1. Error rate

This version of CV \(M\)-time repetitions of the conventional CVK above. In every repetition there is a new randomized partition function \(\mathcal{X}_m(i) = \mathcal{X}(\mathcal{R}_m(i))\), where \(\mathcal{X}\) is defined in (5) and \(\mathcal{R}_m\) is the \(m^\text{th}\) one-to-one randomized mapping of \([i, \ldots, n]\) onto itself. Simply in words, the same conventional partitioning of the CVK is applied each iteration after randomly shuffling the dataset. The training sets, then, are defined for each iteration \(m\) as \(\mathbf{X}_m([k]\mathbf{X}_m([k]))\) \(x \in \mathcal{X}\) \(\mathcal{R}_m(i) \neq k\). The conventional (one run) CVK follows naturally from the CVKR by setting \(M = 1\) and then dropping the subscript \(m = 1\) to
simplify notation. Each repetition, the classifier is trained and tested using the conventional CVK; the scores are stored for all \( n \) observations. The average is taken over all \( M \times n \) scores. The CVKR estimator is defined formally as:

\[
\bar{\text{Err}}^{(CVKR)} = \frac{1}{n} \sum_{i=1}^{n} \left[ \frac{1}{M} \sum_{m=1}^{M} Q \left( x_i, X_{(i)}, m \right) \right].
\]  
(11)

The “stared” variant of the CVKR, where average is taken over repetitions is defined as:

\[
\bar{\text{Err}}^{(CVKR*)} = \frac{1}{M} \sum_{m=1}^{M} \left[ \frac{1}{K} \sum_{k=1}^{K} \frac{1}{n K} \sum_{i \in \mathcal{X}_k} Q \left( x_i, X_{(k)}, m \right) \right] \]
(12a)

\[
= \frac{1}{M} \sum_{m=1}^{M} \left[ \frac{1}{n} \sum_{i=1}^{n} Q \left( x_i, X_{(i)}, m \right) \right]
\]
(12b)

\[
= \frac{1}{n} \sum_{i=1}^{n} \left[ \frac{1}{M} \sum_{m=1}^{M} Q \left( x_i, X_{(i)}, m \right) \right]
\]
(12c)

\[
= \bar{\text{Err}}^{(CVKR)}.
\]
(12d)

Hence, the two variants (11)–(12a) are equivalent. So it does not really matter whether we do: (1) calculating the statistic from the averages-over-randomized-runs for every observation, (2) averaging over the statistic calculated from every partition of every run, or (3) averaging over randomized-runs for the statistic from every run. However, we adopt the first definition (11) for the sake of establishing the comparison in Section 3.1.

Some practitioners estimate the variance from the estimates obtained from each partition/run, similar to the practice for the CVK. As was mentioned above, we defer analysis of variance to another research (Section 5). However, we think that this will exhibit high bias since all of these repetitions are correlated.

2.3.2. AUC

With stratification, we can define the two partitions, using compact notation, as: \( \mathcal{X}_{cm}(i) = \mathcal{X}(\mathcal{X}_{cm}(i)), \ c = 1, 2 \) for the two classes respectively, where \( \mathcal{X} \) is given by (5) and \( \mathcal{X}_{cm} \) is the randomized function, defined above, for class \( c \). The training sets are given by \( X_{c(k),m} = \{ x_i : \mathcal{X}_{cm}(i) \neq k, \ x_i \in X_c \} \). Then, the CVKR estimator is defined for the AUC as:

\[
\bar{AUC}^{(CVKR)} = \frac{1}{n_1 n_2} \sum_{j=1}^{n_1} \sum_{i=1}^{n_2} \left[ \frac{1}{M} \sum_{m=1}^{M} \psi \left( h(x_i), h(y_j) \right) \right], \quad \psi = h x_1_{(i,m)} x_2_{(m)}.
\]

The "stared" variant is defined as:

\[
\bar{AUC}^{(CVKR*)} = \frac{1}{M} \sum_{m=1}^{M} \left[ \frac{1}{K} \sum_{k_1=1}^{K} \sum_{k_2=1}^{K} \frac{1}{n_1 K n_2 K} \sum_{i \in \mathcal{X}_{cm}(k_1)} \sum_{j \in \mathcal{X}_{cm}(k_2)} \psi \left( h(x_i), h(y_j) \right) \right], \quad \psi = h x_1_{(i,m)} y_{(j)}.
\]

The same comments made above for the error rate CVKR estimator are immediate here.

2.4. Monte-Carlo (MC) K-fold CV (CVKM)

2.4.1. Error rate

CVKM is similar to CVKR except in that, in every repetition (called in literature MC run/trial) there is only one partition to test on; i.e., there is only one training set of size \( n - n_K \), and one testing set of size \( n_K \). To be able to formalize and analyze this CVKM version of the Cross Validation we proceed as follows. We index this single testing partition with \( k = 1 \); i.e., testing is carried out only on the first partition. This is without loss of generality since in each MC trial the observations are randomized. Therefore, the training set is \( X_{(1),m} \); which, obviously, may or may not include an observation \( x_i \). Define \( I_i^m = I_{(\mathcal{X}_{cm}(i) = 1)} \), a zero-one condition for testing whether an observation \( x_i \) appears in the testing partition (of \( k = 1 \) or not. We did not need this condition in CVKR, since every MC trial includes \( K \) different training and testing sets and for every \( x_i \) there is a corresponding test set \( X_{(i)}(m) \) that does not include it. It is clear that \( \sum_i I_i^m = n_K \), the number of observations in each, and hence in the first, partition. The CVKM estimator can then be formally defined as:

\[
\bar{\text{Err}}^{(CVKM)} = \frac{1}{n} \sum_i \left[ \sum_{m=1}^{M} Q \left( x_i, X_{(1),m} \right) / \sum_{m=1}^{M} I_i^m \right],
\]

(15)
which means that for every observation we train once and test on that observation if it is not included in the training set. We could have defined the MC estimator so that for every MC loop we train once and test on all of the observations in the testing set; then we average over the MC loops. This “stared” variant should be defined as:

\[
\overline{\text{Err}}^{(CVKM\ast)} = \frac{1}{M} \sum_{m=1}^{M} \left[ \frac{1}{n_K} \sum_{i \in X_m^{(1)}} Q\left(x_i, X_{(i),m}\right) \right]
\]

(16a)

\[
= \frac{1}{M} \sum_{m=1}^{M} \left[ \frac{1}{n_K} \sum_{i} I_m^{\text{err}} \left( x_i, X_{(i),m}\right) \right]
\]

(16b)

\[
= \frac{1}{n} \sum_{i} \left[ \left( \frac{1}{n_K} \sum_{m} I_m^{\text{err}} \left( x_i, X_{(i),m}\right) \right) \right] \rightarrow \overline{\text{Err}}^{(CVKM)}
\]

(16c)

In contrast to the CVN, CVK, and CVKR, the two variants \(\overline{\text{Err}}^{(CVKM)}\) (15) and \(\overline{\text{Err}}^{(CVKM\ast)}\) (16a) are not identical with finite \(M\). However, from the S.L.L.N, we know that \(\frac{1}{n} \sum_{m} I_m^{\text{err}} \rightarrow \mathbb{E} \left[ I_m^{\text{err}} \right] = \frac{n_K}{n}\) as \(M \rightarrow \infty\). Hence, both variants are asymptotically the same and we adopt the first for the sake of establishing the comparison with other CV versions in Section 3.1.

It is worth mentioning that the two variants are very similar (conceptually) to the two variants of the bootstrap (the leave-one-out and the “stared” variant), as discussed in Section 2.5.

2.4.2. AUC

With stratification, as usual, for each MC run there is only single partition from each class to test on. As above, for formalizing and analyzing this variant, W.L.O.G. we set the two testing partitions as \(k_1 = k_2 = 1\). The training sets are therefore \(X_{(i),m}\), \(c = 1, 2\). We define, as well, \(I_{m}^{i} = I_{(x_{im}(i);1)}\) and \(I_{m}^{c} = I_{(x_{im}(j);1)}\). Then, the CVKM variant for the AUC is defined as

\[
\widetilde{AUC}^{(CVKM)} = \frac{1}{n_1 n_2} \sum_{i} \left[ \sum_{m} I_{m}^{i} \psi\left( h(x_i), h(y_j) \right) / \sum_{m} I_{m}^{i} \right], \quad h = h_{x_{1}(i),m} x_{2}(i,m)
\]

(17)

Similar to the treatment above of the error rate, we could have defined this variant as

\[
\overline{\text{AUC}}^{(CVKM\ast)} = \frac{1}{M} \sum_{m=1}^{M} \left[ \frac{1}{n_1 K n_2 K} \sum_{j \in X_m^{(1)}} \sum_{j \in X_m^{(1)}} \psi\left( h(x_i), h(y_j) \right) \right], \quad h = h_{x_{1}(i),m} x_{2}(i,m)
\]

(18a)

\[
= \frac{1}{M} \sum_{m=1}^{M} \left[ \frac{1}{n_1 K n_2 K} \sum_{j} \sum_{j} I_{m}^{i} \psi\left( h(x_i), h(y_j) \right) \right], \quad h = h_{x_{1}(i),m} x_{2}(i,m)
\]

(18b)

\[
= \frac{1}{n_1 n_2} \sum_{i} \left[ \frac{1}{M n_1 K n_2 K} \sum_{m} I_{m}^{i} \sum_{m} I_{m}^{i} \psi\left( h(x_i), h(y_j) \right) / \sum_{m} I_{m}^{i} \right], \quad h = h_{x_{1}(i),m} x_{2}(i,m)
\]

(18c)

The same comment made above on the CVKR variant for the error rate is immediate here; the two variants are not equal for finite \(M\). However, asymptotically \(\frac{1}{M} \sum_{m} I_{m}^{i} \sum_{m} \rightarrow \mathbb{E} \left[ I_{m}^{i} \right] = \frac{n_1 K n_2 K}{n_1 n_2}\) as \(M \rightarrow \infty\). Hence, the two variants are equivalent as \(M \rightarrow \infty\). We adopt the first for the same reason above.

2.5. Leave-One-Out Bootstrap (LOOB)

Bootstrap has a strong connection to, and its literature shares the same variants with, the cross validation; hence, we treat here.

2.5.1. Error rate

The LOOB estimator for the error rate was motivated by Efron in Efron (1983); Efron and Tibshirani (1997) and defined as:

\[
\overline{\text{Err}}^{(1)} = \frac{1}{n} \sum_{i=1}^{n} I_{b}^{i} Q\left( x_i, X^b \right) / \sum_{b} I_{b}^{i}
\]

(19)

where \(I_{b}^{i}\) equals 1 if the observation \(x_i\) did not appear in the bootstrap \(b\) and 0 otherwise; this is to avoid the bias occurring from training and testing on the same observations. The classifier is trained on the \(b^{th}\) bootstrap \(X^b\) and tested on the observation \(x_i\); the procedure is repeated for \(B\) bootstraps. Suppose \(\frac{1}{B} \sum_{b} Q\left( x_i, X^b \right) \rightarrow \text{err}^{f}\) as \(B \rightarrow \infty\), which means that
with increasing the number of bootstrap infinitely the average converges to some function of \( x_i \), named \( \text{err}^i \), which is an estimate of the population error rate of the observation \( x_i \). Then, by Lemma 1, \( \frac{1}{n} \sum b \frac{I^b_i Q(x_i, X^b)}{\sum b I^b_i} \xrightarrow{a.s.} \text{err}^i \) as well, and hence
\[
\overline{E}_{\text{err}}^{(1)} \xrightarrow{a.s.} \frac{1}{n} \sum \text{err}^i, \quad \text{as } B \to \infty.
\] (20)

On the other hand, the definition introduced in Efron and Tibshirani (1993) follows the same motivation of Efron (1983), i.e., testing on those observations not included in the training set. However, it averages over the bootstraps rather than observations. It was introduced this way to provide an analogue to the partitioned ("stared") variant of the CVK:
\[
\overline{E}_{\text{err}}^{(s)} = \frac{1}{B} \sum b \left[ \sum \frac{I^b_i Q(x_i, X^b)}{\sum I^b_i} \right]
\]
(21a)
\[
= \frac{1}{n} \sum b \left( \frac{n}{a^b} \right) Q(x_i, X^b)
\] B.
(21b)

where \( a^b = \sum I^b_i \). From Corollary 3, \( I^b_i \) is a \( Ber \left( \frac{n-1}{2n-1} \right) \) r.v. \( \forall i \). Both variants, (19) and (21a), estimate the expectation (over the training and testing sets) of the error rate, but with different summation order (one sums first over the observations and the other sums first over the bootstraps). Both variants establish the parallelism with the CV variants of previous sections.

Similar to the CVKM, it is obvious that the two variants are not equal for finite bootstraps \( B \); and by comparing equations (19) and (21a), they can be seen as summation with different weights. To analyze them we denote \( \frac{n}{a^b} \) by \( w^b_i \); then direct application of Lemma 1 gives
\[
\overline{E}_{\text{err}}^{(s)} \xrightarrow{a.s.} \frac{1}{n} \sum b \mathbb{E} \left[ w^b_i \text{err}^i \right] = \mathbb{E} \left[ w^b_i \left( \frac{1}{n} \sum \text{err}^i \right) \right]
\] (22)

This means that the ratio between the two estimators (as \( B \to \infty \)); (1) does not depend on the classifier rather it depends on the sampling mechanism (exactly as was the case for the CVKM). (2) The two estimators are not equal even asymptotically with \( B \). From Lemma 4
\[
\overline{E}_{\text{err}}^{(s)} \xrightarrow{a.s.} \left( \frac{2n-2}{2n-1} \right) \frac{1}{n} \sum \text{err}^i \quad \text{as } B \to \infty.
\] (23)

Since the LOOB estimator is a smooth variant in contrast to the "stared" one—for more details on smoothness issue see (Efron and Tibshirani, 1997; Yousef et al., 2005; Yousef, 2019)—we prefer the former in favor of the latter, and send it to Section 3.1 for comparison with other estimators.

2.5.2. AUC

The two variants of the bootstrap estimator for the AUC, that are analogue to those of (19) and (21a) for the error rate, were introduced and defined in our work Yousef et al. (2004, 2005); Yousef (2019) respectively. In those articles, we analyzed their variance and compared them among other bootstrap techniques. In this Section, we provide the theoretical comparison between both variants in parallel to Sections 2.1–2.4. With stratification, we had defined the leave-pair-out bootstrap (LPOBS) for the AUC as:
\[
\overline{\text{AUC}}^{(1,1)} = \frac{1}{n_1 n_2} \sum j \sum b \frac{I^b_i I^b_j \psi(h(x_i), h(y_j))}{\sum b I^b_i I^b_j}, \quad h = h_{X^b}.
\] (24)

Suppose \( \frac{1}{B} \sum b \psi(h(x_i), h(y_j)) \xrightarrow{a.s.} \text{AUC}^{i-j} \) as \( B \to \infty \), \( h = h_{X^b} \), which means that with increasing the number of bootstrap infinitely the average converges to some function of \( x_i \) and \( y_j \), named \( \text{AUC}^{i-j} \), which is an estimate for the population MannWhitney statistic of the observations \( x_i \) and \( y_j \). Since \( I^b_i I^b_j \) is Bernoulli r.v., by Lemma 1, \( \frac{1}{n_1 n_2} \sum j \sum \text{AUC}^{i-j} \xrightarrow{a.s.} \text{AUC}^{i-j} \), \( h = h_{X^b} \), and hence
\[
\overline{\text{AUC}}^{(1,1)} \xrightarrow{a.s.} \frac{1}{n_1 n_2} \sum \sum \text{AUC}^{i-j} \quad \text{as } B \to \infty.
\] (25)
On the other hand, we had defined the "stared" variant for the AUC (Yousef et al., 2004; Yousef, 2019) as

$$\overline{\text{AUC}}^{(s)} = \frac{1}{B} \sum_{b} \left[ \sum_{j} \sum_{i} I_{i}^{b} I_{j}^{b} \psi(h_{X^{+}}(x_i), h_{X^{+}}(y_j)) / \sum_{j} \sum_{i} I_{i}^{b} I_{j}^{b} \right]$$

(26a)

$$= \frac{1}{n_1 n_2} \sum_{j} \sum_{i} \left( \frac{n_1 n_2 I_{i}^{b} I_{j}^{b}}{A_b} \right) \psi(h_{X^{+}}(x_i), h_{X^{+}}(y_j)) \right]$$

(26b)

where $A_b = \sum_j \sum_i I_{i}^{b} I_{j}^{b} = \sum_i I_{i}^{b} \sum_j I_{j}^{b}$. Arranging gives

$$\frac{n_1 n_2 I_{i}^{b} I_{j}^{b}}{A_b} = \frac{n_1 I_{i}^{b}}{\sum_i I_{i}^{b}} \frac{n_2 I_{j}^{b}}{\sum_j I_{j}^{b}} = w_b w'_b,$$

(27)

where $w_b$ and $w'_b$ are independent because of stratification. Then, again by Lemma 1

$$\overline{\text{AUC}}^{(s)} \text{ a.s.} \frac{1}{n_1 n_2} \sum_{j} \sum_{i} E[w_b w'_b] \text{ AUC}^{i,j} = E[w_b] E[w'_b] \left( \frac{1}{n_1 n_2} \sum_{j} \sum_{i} \text{ AUC}^{i,j} \right)$$

(28)

$$= \left( \frac{2n_1 - 2}{2n_1 - 1} \right) \left( \frac{2n_2 - 2}{2n_2 - 1} \right) \left( \frac{1}{n_1 n_2} \sum_{j} \sum_{i} \text{ AUC}^{i,j} \right).$$

Same conclusion and comment made for the error rate variants above are due here. The two variants are not equal even asymptotically with the number of bootstraps $B$. And as was exactly commented at the end of the previous section for the error rat, since $\overline{\text{AUC}}^{(1;1)}$ is a smooth estimator as opposed to $\overline{\text{AUC}}^{(s)}$, we prefer it and send it to Section 3.1 for comparison.

3. Theoretical Critique

3.1. Understanding the Connection Among These Estimators

In the previous section, we formalized the different variants used in the literature by practitioners of each estimator. For some estimators, e.g., CVN, CVK, and CVKR, we found that the variants of each estimator are always equivalent. For CVKM estimator, the variants are equal only asymptotically with the number of MC trials. For the BS estimator, the variants are different even asymptotically with the number of bootstrap replications; however, the LOOB variant, which has the outer summation being over the observations (the pooled variant), is a smooth statistic and is preferred over the other variant. Having said all of that, it is then reasonable to bring here in this section the pooled variant of each estimator to put them side by side for the sake of formalizing the connection among these estimators. We start by the error rate estimators, and same discussion will be immediate for the AUC estimators.

The pooled variant of each error rate estimator (CVN (3), CVK (6), CVKR (11), CVKM (15), and LOOB (19)), are re-listed below respectively:

$$\overline{\text{Err}}^{(CVN)} = \frac{1}{n} \sum_{i=1}^{n} \left[ Q(x_i, X_{(i)}) \right].$$

(30a)

$$\overline{\text{Err}}^{(CVK)} = \frac{1}{n} \sum_{i=1}^{n} \left[ Q(x_i, X_{(i)}) \right].$$

(30b)

$$\overline{\text{Err}}^{(CVKR)} = \frac{1}{n} \sum_{i=1}^{n} \left[ \sum_{m} Q(x_i, X_{(X_{(m)},0)}, M) / M \right].$$

(30c)

$$\overline{\text{Err}}^{(CVKM)} = \frac{1}{n} \sum_{i=1}^{n} \left[ \sum_{m} Q(x_i, X_{(i)}, M) / \sum_{m} I_{m}^{i} \right].$$

(30d)

$$\overline{\text{Err}}^{(1)} = \frac{1}{n} \sum_{i=1}^{n} \left[ \sum_{b} I_{b}^{i} Q(x_i, X_{b}) / \sum_{b} I_{b}^{i} \right].$$

(30e)

After dismissing the other variants of each of these five estimators, we proceed more and show that the CVKM estimator (30d) is, itself, a redundant slower version of the CVKR estimator (30c), and hence should be dismissed as well. This conclusion is immediate by comparing these two equations, if $\sum_{m} Q(x_i, X_{(X_{(m)},0)}, M) / M$ converges a.s. as $M \rightarrow \infty$ then by Lemma 1, $\sum_{m} I_{m}^{i} Q(x_i, X_{(i)}, M) / \sum_{m} I_{m}^{i}$ converges, as well, a.s. to the same value. Hence, these two versions of CV produces the same estimate as $M \rightarrow \infty$. However, $I_{m}^{i}$ is $\text{Ber}(n K/n)$, which of course delays the convergence. Said differently, if compared to CVKM, CVKR is less noisier at finite $M$, and hence, more favorable; and practitioners should be
discouraged from using CVKM. This leaves us with a less noisier literature with only three CV estimators, (30a)–(30c), and the LOOB estimator, (30e).

On the other hand, the AUC estimators: CVN (4), CVK (8), CVKR (13), CVKM (17), and LOOB (24), are listed below respectively.

\[
\hat{AUC}^{(CVN)} = \frac{1}{n_1 n_2} \sum_{j=1}^{n_2} \sum_{i=1}^{n_1} \psi[h(x_i), h(y_j)], \quad h = h_{X_1, y, X_2}.
\]

\[
\hat{AUC}^{(CVK)} = \frac{1}{n_1 n_2} \sum_{j=1}^{n_2} \sum_{i=1}^{n_1} \psi[h(x_i), h(y_j)], \quad h = h_{X_1, y, X_2}.
\]

\[
\hat{AUC}^{(CVKR)} = \frac{1}{n_1 n_2} \sum_{j=1}^{n_2} \sum_{i=1}^{n_1} \left[ \frac{\sum_{m} I_{jm} I_{jm} \psi[h(x_i), h(y_j)]}{\sum_{m} I_{jm} I_{jm}} \right], \quad h = h_{X_1, y, X_2}.
\]

\[
\hat{AUC}^{(CVKM)} = \frac{1}{n_1 n_2} \sum_{j=1}^{n_2} \sum_{i=1}^{n_1} \left[ \sum_{b} I_{ib} I_{ib} \psi[h(x_i), h(y_j)] / \sum_{b} I_{ib} I_{ib} \right], \quad h = h_{X_1, y, X_2}.
\]

By observing that \( I_{jm} I_{jm} \) in (31d) and \( I_{ib} I_{ib} \) in (31e) each is Bernoulli r.v.; and a conclusion identical to that following (30) for the error rate estimators is immediate here for the AUC estimators. This is obvious since that conclusion is inherent in the resampling mechanism rather than the estimated measure.

Now, we have four estimators, or resampling mechanisms, remaining after the filtration of the previous and current sections: CVN, CVK, CVKR, and LOOB that appear in (30) and (31) for the error rate and AUC respectively. It is important to emphasize that these estimators were long standing in the literature and have been numerically compared in many studies including the early seminal work by Efron and Tibshirani (Efron and Tibshirani, 1997). Conducting another computational comparative study, that considers new distributions and real datasets than those considered in the literature, is quite out of scope and objective of the present article and we defer it to another article. However, a few remarks are in order for the sake of completeness as long as we put them side by side. These remarks are discussed below.

3.2. Conditional vs. Mean Performance

CVN (30a) and CVK (30b) (and exactly similarly for their AUC analogues (31a) and (31b)) are the only versions that do not average over training sets for every observation. The error from testing on \( x_i \) is produced solely by training once on \( X_{(i)}, \) or \( X_{(i)} \) respectively. Hence, they can be seen as if they were designed to estimate the conditional performance \( Err_{X} = E_{x}(Q(x, X)|x, X) \) of the classification rule; i.e., the performance conditional on the training set \( X \). This is with possibly more anticipated bias for CVK than CVN since their effective training set size are \( n - n/K \) and \( n - 1 \) respectively.

On the other hand both, CVKR (30c) and LOOB (30e), average over many training sets (MC or bootstraps) to produce one error estimate per observation, i.e., \( \sum_{m} Q(x_i, X_{(X_{(i)}, m)}) / M \) and \( \sum_{b} I_{i} I_{b} Q(x_i, X^b) / \sum_{b} I_{i} I_{b} \) respectively. Hence, they can be seen as if they are designed to estimate the unconditional performance \( E_{rr} = E_{X}(Err_{X} = E_{X}E_{X}(Q(x, X)|x, X)) \) of the classification rule; i.e., the expected conditional performance, where the expectation is taken over the population of training sets of the same size \( n \). Efron and Tibshirani (1997) call LOOB, and for the same reason we can call CVKR, a smooth version of CVN since the error for every observation \( x_i \) is calculated from averaging over many training sets. Both estimators are setting on an underlying layer of cross validation. However, the two estimators differ in their mechanism of averaging over the training sets. The CVKR estimator partitions the training set equally. It gives the same chance to all observations in the training sets to appear in the repeated MC sampling (including an outlier that no other observation in the training set is close to it). On contrary, the LOOB estimator samples, with replacement, from the MLE distribution (the empirical distribution; or said differently, the apparent distribution). This gives more chance to close-to-each-other observations to appear in the bootstraps than other distant-from-each-other observations, which mimics the true distribution. Although both the CVN and CVK look, in theory, like estimating the conditional performance whereas the CVKR and LOOB look like estimating the mean performance, all, in practice, do estimate the mean performance! This is a consequence of the known phenomenon of “weak correlation” that we illustrate below both mathematically and numerically.

3.3. Components of Variance of Performance Estimators and Weak Correlation

Many simulation results, e.g., Efron (1983; Efron and Tibshirani (1997), show that there is only a very weak correlation between the cross validation estimator and the conditional true error rate \( Err_{X} \). This issue is discussed in mathematical detail in the excellent paper by Zhang (1995), which therefore concludes that the cross-validation estimator should not be used to estimate the true error rate of a classification rule conditional on a particular training data set. Other estimators discussed above have this same attribute, since they have the same resampling ingredient of the CV estimator and “we would guess, for any other estimate of conditional prediction error” (Sec. 7.12, Hastie et al., 2009). We provide our simple mathematical elaboration below.
Denote the true performance of the classification rule conditional on the training set $X$ (whether $Err_X$ or $AUC_X$) by $S_X$, the unconditional performance by $E_X S_X$, and an estimator of either of them by $\hat{S}_X$. For easier notation we can unambiguously drop the subscript $X$ and decompose the MSE as:

$$
\text{MSE}(\hat{S}, S) = E(\hat{S} - S)^2
= E(\hat{S} - E S)^2 + \text{Var}(S) - 2 \text{Cov}(\hat{S}, S).
$$

By normalizing with the standard deviations we get:

$$
\frac{\text{MSE}(\hat{S}, S)}{\sigma_S \sigma_{\hat{S}}} = \frac{\text{MSE}(\hat{S}, E S)}{\sigma_S \sigma_{\hat{S}}} + \frac{\sigma_S}{\sigma_{\hat{S}}} - 2 \rho_{SS}.
$$

This equation relates four crucial components to each other:

- $\text{MSE}(\hat{S}, S)/\sigma_S \sigma_{\hat{S}}$, the normalized MSE of $\hat{S}$ if it is seen as an estimator of the conditional performance $S$.
- $\text{MSE}(\hat{S}, E S)/\sigma_S \sigma_{\hat{S}}$, the normalized MSE of $\hat{S}$ if it is seen as an estimator of the expected performance $E S$ (and therefore called MSE around the mean).
- $\sigma_S/\sigma_{\hat{S}}$, the standard deviation ratio between $S$ and $\hat{S}$.
- $\rho_{SS}$, the correlation coefficient between $S$ and $\hat{S}$.

From (33), an estimator $\hat{S}$ is a good candidate to estimate $S$ than $E S$ if its $\text{MSE}(\hat{S}, S)$ is less than its $\text{MSE}(\hat{S}, E S)$. Then, it is the responsibility of the correlation coefficient $\rho_{SS}$ to be high enough to cancel $\sigma_S/\sigma_{\hat{S}}$ and a portion of $\text{MSE}(\hat{S}, E S)$. Unfortunately, this does not happen as will be experimentally illustrated in Section 4 below.

4. Experiments

We elaborate experimentally on the concept of weak correlation discussed above by a very simple toy example. We generate a five dimensional ($p = 5$) multinormal 2-class data with identity covariance matrices with mean vectors of $\mathbf{0}$ and $c \mathbf{1}$. It is known that the Mahalanobis distance between the two classes, defined as $\Delta = [(\mu_1 - \mu_2)' \Sigma^{-1} (\mu_1 - \mu_2)]^{1/2}$, is given by $\Delta = c^2 p$ for the multinormal distributions. Therefore, 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 used is 1000.

Table 1 provides all quantities of (33) of these experiments under different values of training sample size $n$. It is obvious from the values that $\text{RMS}(\hat{S}, S)$ and $\text{RMS}(\hat{S}, E S)$ are very close to each other because of that the quantity $\sigma_S/\sigma_{\hat{S}} - 2 \rho_{SS} \approx 0.413 - 2 \times 0.290 = -0.167$ (on average over the 10 experiments shown in the table); and in some cases, e.g., the first experiment it goes low as $-0.052$. For short, the correlation between $\hat{S}$ and $S$ is weak to cast $\hat{S}$ as an estimate to $S$ even though it is designed to estimate it!

For more illustration, Figure 1 visualizes the components in the decomposition (33) and the numbers in Table 1. This figure shows 15 realizations of the 1000 MC trials of the same experiment above. On the right are the true values of $S$ when trained on these different 15 training sets. On the left are the corresponding 15 estimated values of $\hat{S}$. The lines provide links between the true values and the corresponding estimates. This figure shows that two nearby true values of $S$ are likely to have two widely separated estimated values $\hat{S}$ on different sides of the mean. This visually illustrates the lack of correlation (or the weak correlation) between the estimators and the true conditional performance.

5. Conclusion, Discussion, and Suggested Future Work

We analyzed many versions of cross validation used by practitioners in the literature, and different variants of each version. In addition, we analyzed some of the bootstrap based estimators for their strong connection to the cross validation, to have one blueprint of all of them. We found that many variants are equivalent; whereas others are not smooth, the matter that disqualifies them from further variance analysis using sophisticated mathematical procedures, e.g., like the Influence Function (IF). Therefore, these variants should be abandoned to have more quiet (as opposed to noisy) literature. We filtered all of them and came up with only one variant of each version. Further, we put side-by-side these versions for better understanding of how they agree or differ. After the unified mathematical formalization of all of them, it became clear that both leave-one-out (CVN) and $K$-fold cross validation (CVK) look like estimating the conditional performance of a classification rule; whereas repeated $K$-fold cross validation (CVKR) and monte-carlo cross validation (CVKM) look like estimating the mean (over different training sets) performance of the classification rule, with slower convergence rate of the latter; hence abandoned as well. We therefore ended up with just three estimators, the CVN, CVK, and CVKR, and suggest that practitioners drop any other version or variant to stop confusing the community and literature.

We went further by explaining the weak correlation issue, both mathematically and numerically by a simple set of experiments. We illustrated that using either the CVN or CVK version, which look mathematically like as if they are designed...
| $\hat{S}$ | E   | $\sigma$ | RMS($\hat{S}, S$) | RMS($\hat{S}, E.S$) | $\rho_{\hat{S}, S}$ | $n$ |
|------|------|---------|------------------|------------------|------------------|-----|
| $S$  | 0.6181 | 0.0434  | 0                | 0.0434           | 1.0000           |     |
| $\tilde{S}$ | 0.8897 | 0.0475  | 0.2774           | 0.2757           | 0.2231           | 20  |
| $\hat{S}$ | 0.5914 | 0.0947  | 0.0973           | 0.0984           | 0.2553           |     |
| $S$  | 0.6231 | 0.0410  | 0                | 0.0410           | 1.0000           |     |
| $\tilde{S}$ | 0.8788 | 0.0499  | 0.2615           | 0.2606           | 0.2991           | 22  |
| $\hat{S}$ | 0.5945 | 0.0947  | 0.0956           | 0.0990           | 0.2993           |     |
| $S$  | 0.6308 | 0.0400  | 0                | 0.0400           | 1.0000           |     |
| $\tilde{S}$ | 0.8656 | 0.0471  | 0.2406           | 0.2395           | 0.2833           | 25  |
| $\hat{S}$ | 0.5991 | 0.0865  | 0.0897           | 0.0922           | 0.2946           |     |
| $S$  | 0.6359 | 0.0338  | 0                | 0.0358           | 1.0000           |     |
| $\tilde{S}$ | 0.8554 | 0.0472  | 0.2253           | 0.2246           | 0.2747           | 28  |
| $\hat{S}$ | 0.6035 | 0.0840  | 0.0874           | 0.0901           | 0.2904           |     |
| $S$  | 0.6469 | 0.0343  | 0                | 0.0343           | 1.0000           |     |
| $\tilde{S}$ | 0.8419 | 0.0439  | 0.2010           | 0.1999           | 0.2434           | 33  |
| $\hat{S}$ | 0.6170 | 0.0750  | 0.0792           | 0.0807           | 0.2746           |     |
| $S$  | 0.6571 | 0.0308  | 0                | 0.0308           | 1.0000           |     |
| $\tilde{S}$ | 0.8246 | 0.0431  | 0.1735           | 0.1730           | 0.2923           | 40  |
| $\hat{S}$ | 0.6244 | 0.0711  | 0.0753           | 0.0783           | 0.3185           |     |
| $S$  | 0.6674 | 0.0271  | 0                | 0.0271           | 1.0000           |     |
| $\tilde{S}$ | 0.8091 | 0.0406  | 0.1473           | 0.1474           | 0.3517           | 50  |
| $\hat{S}$ | 0.6357 | 0.0654  | 0.0690           | 0.0727           | 0.3534           |     |
| $S$  | 0.6808 | 0.0217  | 0                | 0.0217           | 1.0000           |     |
| $\tilde{S}$ | 0.7946 | 0.0355  | 0.1195           | 0.1192           | 0.2499           | 66  |
| $\hat{S}$ | 0.6533 | 0.0546  | 0.0602           | 0.0611           | 0.2451           |     |
| $S$  | 0.6965 | 0.0158  | 0                | 0.0158           | 1.0000           |     |
| $\tilde{S}$ | 0.7772 | 0.0312  | 0.0860           | 0.0866           | 0.3596           | 100 |
| $\hat{S}$ | 0.6738 | 0.0454  | 0.0483           | 0.0507           | 0.3422           |     |
| $S$  | 0.7141 | 0.0090  | 0                | 0.0090           | 1.0000           |     |
| $\tilde{S}$ | 0.7573 | 0.0228  | 0.0487           | 0.0489           | 0.2277           | 200 |
| $\hat{S}$ | 0.6991 | 0.0298  | 0.0327           | 0.0334           | 0.2288           |     |

Table 1: A sample from a large set of experiments that shows true performance $S$, apparent performance on the same training set $\tilde{S}$, and estimator $\hat{S}$ from equations (30) or (31). (The typical values in this table are for $S = AUC_X$ and $\hat{S} = \tilde{AUC}_{\hat{X}}^{(\hat{S})}$. The table illustrates weak correlation between $S$ and $\hat{S}$.)

Figure 1: The lack of correlation (or the very weak correlation) between the bootstrap-based estimators and the true conditional performance. Every line connects the true performance of the classifier trained on a data set $X_i$ and the estimated value. The figure represents 15 trials of the 1000 MC trials. Two nearby values of true performance may correspond to two widely separated estimates on different sides of the mean.
to estimate the conditional performance, almost estimate, in terms of the RMS error, the mean performance. However, this leaves us with a question that is still not answered yet: what is the final advice for practitioners regarding which version of the three should be used? The answer to this question may be provided via one of the following two suggested research points.

5.1. Comprehensive Comparative Study

A very comprehensive computational study that supports many distributions, real datasets, classifier architectures, etc., to compare among the relative accuracy of these three estimators is missing. This is, all the more, true after the new era of deep learning and the very complex classifiers they produce. The current studies available in the literature show that there is no overall winner in terms of RMS value. Such a comprehensive computational study is currently under our consideration.

5.2. A Rigorous Method for Estimating the Standard Error of The Three Versions

Is it possible to construct a rigorous method that estimates the standard error of any of these three versions? What is available in the literature is a set of ad-hoc procedures that estimate the variance of the CVK from the $K$ folds, neglecting with that the covariance structure among them. In that regard, Bengio and Grandvalet (2004) concludes that “No Unbiased Estimator of the Variance of K-Fold Cross-Validation". One of the possible approaches is to use the Influence Function (IF) approach for estimating the standard error of the CVKR estimator since it is the only smooth version among the three. Although the approach is feasible and has been used, as mentioned earlier, in Efron and Tibshirani (1997) for the LOOB of the error rate and then in our work (Yousef et al., 2005) for the LPOBS of the AUC, the derivation involves mathematical details that vary from estimator to another. Below we sketch this path for the CVKR version that estimates the AUC—which is more tedious than that of the error rate.

For short, we can rewrite (31c) as

$$AUC^{(CVKR)} = \frac{1}{n_1n_2} \sum_{j_2=1}^{n_2} \sum_{j_1=1}^{n_1} \left[ \sum_m \psi(h_m(j_1), h_m(j_2)) / M \right]. \tag{34}$$

Then, following Yousef et al. (2005), it can be rewritten after perturbing the probability measure of the observation $i$ with a measure $\varepsilon$ as

$$AUC^{(CVKR)}_{\varepsilon,i} = \sum_{j_2=1}^{n_2} \sum_{j_1=1}^{n_1} f_{1_{\varepsilon,i}}(j_1) f_{2_{\varepsilon,i}}(j_2) \left[ \sum_m \psi(h_m(j_1), h_m(j_2)) G_{\varepsilon,i} \right] \tag{35a}$$

$$= \sum_{j_2=1}^{n_2} \sum_{j_1=1}^{n_1} A(\varepsilon) B(\varepsilon), \tag{35b}$$

Then, derivatives and mathematical manipulation should be proceeded to come up with a final mathematical expression for the standard error; and experimental study should assess that expression. If such a direction succeeds in estimating the standard error of the CVKR, it will be a big advantage over the other two non-smooth versions.

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7. Appendix

Lemma 1. Consider the sequence of r.v. $\{X_i\}$, where $\sum_i X_i \overset{a.s.}{\rightarrow} S$, and $S$, in general, is a r.v.. Consider, as well, both, the sequence $\{I_i\}$ of independent events, where $I_i \sim Ber(p)$, and the sequence $\{a_i\}$ of discrete i.i.d. r.v. with mean $E[a_1]$. Then,

1. $\sum_i I_i x_1 \overset{a.s.}{\rightarrow} S.$ \tag{36}

2. $\sum_i \frac{I_i x_1}{n} \overset{a.s.}{\rightarrow} pS.$ \tag{37}

3. $\sum_i \frac{a_i x_1}{n} \overset{a.s.}{\rightarrow} E[a_1] S.$ \tag{38}

Proof.
1. Consider the set $J = \{ j : I_j = 1 \}$; then $\sum_i \frac{I_i x_i}{n}$ can be rewritten as $\sum_i \frac{N x_i}{N}$, where $N = |J|$. Then what remains is showing that $N$ is infinite (with the care that $N$ is a r.v.), which leads to that the summation converges a.s. by assumption. Since $\sum_{i=1}^{\infty} P(I_i) = \infty$, then by Borel-Cantelli Lemma $P(I_i \ i.o.) = 1$; or said differently, the set on which $|J|$ is not infinite is a null set; hence the summation $\sum_i \frac{x_i}{N}$ does not converge (because of the reason that $N$ is finite) only on a set with measure zero; hence $\sum_i \frac{I_i x_i}{\sum I_i} \xrightarrow{a.s.} S$.

2. We have by assumption $\sum_i \frac{x_i}{n} \rightarrow_S S$, then $\sum_i \frac{(x_i - S)}{n} = \sum_i \frac{x_i}{n} - S \xrightarrow{a.s.} 0$; and so does $\sum_i \frac{I_i (x_i - S)}{x_i I_i}$ by the first part of the Lemma. Since

$$\left| \frac{1}{n} \sum_{i=1}^{n} I_i (x_i - S) \right| \leq \frac{1}{\sum_{i=1}^{n} I_i} \sum_{i=1}^{n} I_i (x_i - S),$$

then,

$$\left\{ \{\omega \in \Omega : \left| \frac{1}{n} \sum_{i=1}^{n} I_i (x_i - S) \right| > \epsilon \right\} \subseteq \left\{ \{\omega \in \Omega : \left| \frac{1}{\sum_{i=1}^{n} I_i} \sum_{i=1}^{n} I_i (x_i - S) \right| > \epsilon \right\}.$$

But the set of the r.h.s. converges to a null set (by a.s. convergence proved above); hence the l.h.s. converges too to a null set, which concludes that

$$\frac{1}{n} \sum_{i=1}^{n} I_i (x_i - S) \xrightarrow{a.s.} 0.$$  

Then

$$\frac{1}{n} \sum_{i=1}^{n} I_i x_i - S \sum_{i=1}^{n} \frac{I_i}{n} \rightarrow_S 0.$$  

But since $I_i$s are i.i.d. then $\frac{1}{n} \sum_{i=1}^{n} I_i \xrightarrow{a.s.} p$ by SLLN, and by Slutsky’s theorem

$$\frac{1}{n} \sum_{i=1}^{n} I_i x_i \xrightarrow{a.s.} pS.$$  

3. For any discrete r.v. $a$ taking the values $a^j$ with probability $p^j$, $j = 1, \ldots, k$ it can be represented as $a = \sum_j a^j I_{\{\omega : a(\omega) = a^j\}}$, where the sets $\{\omega : a(\omega) = a^j\}$ partition $\Omega$. For simplicity, we can write $a = \sum_j a^j I^j$. Then $a_i = \sum_j a^j I^j_i$, where $I^j_i$, by running the index $i$ and keeping $j$ fixed, are i.i.d. $\text{Ber}(p^j)$. Then

$$\frac{1}{n} \sum_{i=1}^{n} a_i x_i = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{k} a^j I^j_i x_i$$

$$= \sum_{j=1}^{k} a^j \frac{1}{n} \sum_{i=1}^{n} I^j_i x_i.$$  

But we have just proved that $\frac{1}{n} \sum_{i=1}^{n} I^j_i x_i \xrightarrow{a.s.} p^j S$. Then, again by Slutsky’s

$$\frac{1}{n} \sum_{i=1}^{n} a_i x_i \xrightarrow{a.s.} \sum_{j=1}^{k} a^j p^j S = E[a_1] S.$$  

**Lemma 2.** For a bootstrap replication from $n$ observations (with sampling with replacement and without ordering) the quantity $a_{0} = \sum_{i=1}^{n} I^0_i$, where $I^0_i = 1$ if the $i^{th}$ observation does not appear in the replication, has the following properties. (The third point will not be needed later in the analysis but is provided for mathematical interest and completeness)

1. $\Pr[a_{0} = k] = \frac{\binom{n}{k} \binom{n-k}{n-1}}{(\binom{2n-1}{n})}$, $0 \leq k \leq n - 1$,  

2. $E[a_{0}] = \frac{n(n-1)}{2n-1}$,  

3. $E\left[ \frac{1}{1+a_{0}} \right] = \frac{2}{n+1}$.

**Proof.**
1. Bootstrapping a replication can be seen as sampling with replacement without ordering; there are \( \binom{N+K-1}{K} \) different combinations for sampling \( K \) from \( N \) with replacement without ordering; If all of the observations appear in a replication, i.e., \( p_i^b = 1 \) \( \forall i \), then \( a_b = 0 \); and if only one observation appears \( n \) times then \( a_b = n - 1 \). It follows that \( 0 \leq a_b \leq n - 1 \). In general, sampling \( m \) from \( n \) with replacement without ordering will let \( a_b \) take the value \( k \). This \( k \) can be chosen by \( \binom{n}{k} \). The remaining \( n - k \) will appear as is in the \( m \) sampled observations. The rest, i.e., \( m - (n - k) \), will be sampled from the \( n - k \). Hence, \( N = n - k \) and \( K = m + k - n \) and the probability of having \( a_b = k \) is given by

\[
\frac{\binom{n}{k} \binom{m+n-m-k-n}{m-k-n}}{\binom{m+n-1}{m}} = \frac{\binom{n}{k} \binom{m-1}{m-n}}{\binom{m+n-1}{m}}.
\]

(50)

Bootstrapping is a special case, where \( m = n \). What remains is proving that the probabilities add to 1.

\[
(1 + x)^m = (1 + x)^n (1 + x)^{m-n}, \quad \forall x, \quad 0 \leq n \leq m
\]

\[
= \sum_{i=0}^{n} \sum_{j=0}^{m-n} \binom{n}{i} x^i \binom{m-n}{j} x^j.
\]

Then the coefficient of \( x^k \), \( 0 \leq k \leq m \), should match for both sides, which leads to

\[
\binom{m}{k} = \sum_{i=0}^{k} \binom{n}{i} \binom{m-n}{k-i},
\]

(53)

where \( \binom{y}{x} = 0 \) for \( x > y \). If we set \( m = n' + n - 1 \) and \( k = n - 1 \), we have

\[
\binom{n' + n - 1}{n - 1} = \sum_{i=0}^{n-1} \binom{n}{i} \binom{n'-1}{n-1-i}, \quad \text{or}
\]

\[
\binom{n' + n - 1}{n'} = \sum_{i=0}^{n-1} \binom{n}{i} \binom{n'-1}{i+n'-n},
\]

\[
1 = \sum_{i=0}^{n-1} \binom{n}{i} \binom{n'-1}{n'-i}.
\]

(54) (55) (56)

2. For finding the expectation, consider first the identity

\[
(x + y)^n (1 + y)^m = \sum_{i=0}^{n} \binom{n}{i} x^i y^{n-i} \sum_{j=0}^{m} \binom{m}{j} y^j
\]

\[
= \sum_{i=0}^{n} \sum_{j=0}^{m} \binom{n}{i} \binom{m}{j} x^i y^{n-i+j}
\]

(57) (58)

Differentiating both w.r.t. \( x \) then setting \( x = 1 \) gives

\[
n(1 + y)^{m+n-1} = \sum_{i=0}^{n} \sum_{j=0}^{m} \binom{n}{i} \binom{m}{j} y^{n-i+j}
\]

(59)

The coefficient of any power of \( y \) in both sides should agree; hence, matching the coefficient of \( y^n \) in both sides and setting \( m = n - 1 \) gives

\[
n \binom{2n-2}{n} = \sum_{i=0}^{n-1} \binom{n}{i} \binom{n-1}{i}
\]

(60)

Then

\[
E_{a_b} = \sum_{k=1}^{n-1} k \binom{n-1}{k} \binom{m}{k} \binom{n}{2n-2}
\]

\[
= \frac{n^{2n-2}}{2n-1}
\]

(61) (62) (63)
3. Integrating both sides of (58) w.r.t. \(x\), setting \(x = 1\), and setting \(m = n - 1\) gives

\[
\frac{1}{n+1}(1+y)^{2n} = \sum_{i=0}^{n} \sum_{j=0}^{n-1} \frac{1}{i+1} \binom{n}{i} \binom{n-1}{j} y^{n-i+j}.
\] (64)

Then matching the coefficient of \(y^n\) in both sides (by setting \(i = j\) in the R.H.S.) gives

\[
\frac{1}{n+1} \left(\frac{2n}{n}\right) = \sum_{i=0}^{n-1} \frac{1}{i+1} \binom{n}{i} \binom{n-1}{i}.
\] (65)

Then

\[
E\left[\frac{1}{1+a_b}\right] = \frac{1}{(2n-1)} \sum_{i=0}^{n-1} \frac{1}{i+1} \binom{n}{i} \binom{n-1}{i} = \frac{2}{n+1}.
\] (66)

which completes the proof.

\[\blacksquare\]

**Corollary 3 (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.

**Proof.** The statement of this corollary was provided as (Lemma 2 Yousef, 2019) and was proved as follows: 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

\[
1 - \Pr[I_i^b = 1] = 1 - \frac{(n-1) + (n-1)}{\binom{2n-1}{n}} = \frac{n}{2(n-1)} \geq 1.
\] (69)

However, this result is immediate from the above Lemma, where the statement of the corollary could be posed as \(a = \sum_i I_i\); then \(Ea = E\sum_i I_i = \sum_i E I_i = n E I_1 = n \Pr[I_1 = 1]\) (from symmetry of \(I_i\)). Then, \(\Pr[I_1 = 1] = E[a_b/n] = \frac{n-1}{2n-1}\); or \(\Pr[I_1 = 0] = \frac{n}{2n-1}\).

**Lemma 4.** The r.v. \(w_b = \frac{n}{a_b}\) has a mean of \(\frac{2}{n-1}\).

**Proof.** If we denote \(a_b\) by \(a_b^n\) (to resemble sampling from \(n\) observations), then we can say that \(a_b^{n-1} = I_i^b + a_b^n\), in which case \(I_i^b\) and \(a_b^{n-1}\) are independent. Here, \(a_b^{n-1}\) represents sampling from the remaining \(n - 1\) observations having the \(i\)th observation left-out from the bootstrap, i.e., \(I_i^b = 1\). Then,

\[
w_b = \begin{cases} 
0 & \text{if } I_i^b = 0 \\
\frac{n}{1+a_b^n} & \text{if } I_i^b = 1
\end{cases}
\] (71)

where \(0 \leq a_b^{n-1} \leq n - 2\) with pmf given by replacing \(n\) by \(n - 1\) and \(m\) by \(n - 1\) in (50). Then,

\[
E w_b = \Pr[I_i^b = 1] E[w_b | I_i^b = 1]
\] (72)

\[
= \Pr[I_i^b = 1] \frac{n-2}{n} \sum_{i=0}^{n-1} \frac{1}{i+1} \frac{\binom{n-1}{i+1}}{\binom{2n-2}{n}}.
\] (73)

Integrating both sides of (58) w.r.t. \(x\) gives

\[
\frac{1}{n+1}(x+y)^{n+1}(1+y)^m = \sum_{i=0}^{n} \frac{1}{i+1} \binom{n}{i} x^{i+1} y^{n-i} + \frac{1}{n+1} \binom{m}{j+1} y^j,
\] (74)
where the term \( \frac{1}{n+1} y^{n+1} \) is the constant of integration. Setting \( x = 1 \), and setting \( m = n \) gives

\[
\frac{1}{n+1} (1 + y)^{2n+1} = \sum_{i=0}^{n} \sum_{j=0}^{n} \frac{1}{i+1} \binom{n}{i} y^{n-i-j} + \frac{1}{n+1} \sum_{j=0}^{n} \binom{n}{j} y^{n+j}. \tag{75}
\]

Then matching the coefficient of \( y^{n+1} \) in both sides (by setting \( j = i + 1 \) in the double summation and \( j = 0 \) in the single summation) gives

\[
\frac{1}{n+1} \binom{2n+1}{n+1} = \sum_{i=0}^{n-1} \frac{1}{i+1} \binom{n}{i} \binom{n}{i+1} + \frac{1}{n+1} \tag{76}
\]

\[
\sum_{i=0}^{n-1} \frac{1}{i+1} \binom{n}{i} \binom{n}{i+1} = \frac{1}{n+1} \left( \frac{2n+1}{n+1} - 1 \right). \tag{77}
\]

So,

\[
\sum_{i=0}^{n-2} \frac{1}{i+1} \binom{n-1}{i} \binom{n-1}{i+1} = \frac{1}{n} \left( \frac{2n-1}{n} - 1 \right). \tag{78}
\]

Then,

\[
E \frac{w_b}{n} = \frac{n-1}{(2n-1)} \frac{1}{n} \left( \frac{(2n-1)}{2n} - 1 \right) \tag{79}
\]

\[
= \frac{n!}{2(n-1)!} \left[ \left( \frac{2n-1}{2n} \right) - 1 \right] \tag{80}
\]

\[
= \frac{1}{2n-1} \left( \frac{2n-1}{n} - 1 \right) \tag{81}
\]

\[
= 1 - \Pr \{ a_b = 0 \} \tag{82}
\]

\[
= \Pr \{ a_b \neq 0 \}. \tag{83}
\]

The same result could have been obtained by observing that

\[
E \frac{w_b}{n} = \frac{1}{n} \sum_i E \frac{w_b}{i} = \frac{1}{n} \sum_i E \frac{n I^b}{a_b} \tag{84}
\]

\[
= E \frac{I^b}{a_b} \tag{85}
\]

\[
= E \frac{a_b}{a_b} \tag{86}
\]

\[
= \Pr \{ a_b \neq 0 \}. \tag{87}
\]

The last equation follows from that \( \frac{a_b}{a_b} = \text{Ber}(\Pr \{ a_b \neq 0 \}) \).

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