Consistent Cross Validation with Stable Learners

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Abstract

This paper investigates the efficiency of different cross-validation (CV) procedures under algorithmic stability with a specific focus on the K-fold. We derive a generic upper bound for the risk estimation error applicable to a wide class of CV schemes. This upper bound ensures the consistency of the leave-one-out and the leave-p-out CV but fails to control the error of the K-fold. We confirm this negative result with a lower bound on the K-fold error which does not converge to zero with the sample size. We thus propose a debiased version of the K-fold which is consistent for any uniformly stable learner. We apply our results to the problem of model selection and demonstrate empirically the usefulness of the promoted approach on real world datasets.

1 Introduction

Introduced in Stone 1974, cross-validation (CV) is a most popular tool in statistics for estimating the generalization risk of a learning algorithm. It is also the mainstream approach for model and parameter selection. Despite its widespread use, it has been shown in several contexts that CV schemes fail to select the correct model unless the test fraction is negligible in front of the sample size. Unfortunately this excludes the widely used K-fold CV. This sub-optimality for model selection has been pinned in the linear regression framework by Shao 1993, 1997; Yang 2007, then in other specific frameworks such as density estimation (Arlot 2008) and classification (Yang 2006). The theoretical properties of CV procedures for model selection in wider settings are notoriously difficult to establish. One reason for this is the correlation between the rules learned on each fold.

Contrarily to the references cited above our main focus (to the exception of Section 6) is risk estimation, i.e. we investigate the error made by the CV estimator when estimating the generalization risk of a given learning algorithm. Since this problem is in principle easier than model selection, our negative result regarding the standard K-fold CV (a lower bound on the K-fold error, as detailed below) has a somewhat more general scope than existing negative results. In addition contrarily to most previous works our positive results (PAC upper bounds on the error) concern the wide class of stable learning algorithms. Indeed
our working assumption of uniform stability encompasses many algorithms such as Support Vector Machines and Least square regression (Bousquet and Elisseeff 2002), Stochastic Gradient Descent (Hardt et al. 2016) and neural networks with a simple architecture (Charles and Papailiopoulos 2018). The notion of algorithmic stability and its consequences in learning theory has received much attention since its introduction in Devroye and Wagner 1979. This property permits to obtain generalization bounds for a large class of a learning algorithms such as k-nearest-neighbors (Devroye and Wagner 1979), empirical risk minimizers (Kearns and Ron 1999), regularization networks (Bousquet and Elisseeff 2001), bagging (Elisseeff et al. 2005) to name but a few. For an exhaustive review of the different notions of stability and their consequences on the generalization risk of a learning algorithms the reader is referred to Kutin and Niyogi 2002.

Related work on CV risk estimation with stable learners In Kumar et al. 2013, K-fold CV for risk estimation is envisioned under stability assumptions regarding the algorithm. It is shown that the K-fold risk estimate has a much smaller variance than the simple hold-out estimate and the amount of variance reduction is quantified. However, the latter results do not imply a universal upper bound regarding the K-fold neither for risk estimation nor for model selection. Another related work is Celisse and Guedj 2016, who build upon another variant of algorithmic stability, namely \(L^q\)-stability to derive PAC upper bounds for leave-p-out (l.p.o.) error estimates. Other results regarding l.p.o. consistency for stable algorithms can be found in Cornec 2017. For the l.p.o. and the leave-one-out (l.o.o.) these upper bounds are sanity-check bound (Kearns and Ron 1999), which means that they are satisfactory in that they display the usual rate of a PAC generalization bound converging to zero with the sample size \(n\) at rate \(O(1/\sqrt{n})\).

In contrast with the l.p.o. case, to our best knowledge the literature on algorithmic stability is silent about the consistency of K-fold CV – the most widely used CV scheme – in a generic stability setting. Filling this gap is the main purpose of the present paper.

Contributions and outline We introduce the necessary background and notations about CV risk estimation and algorithmic stability in Section 2. Section 3 is intended to give some context about provable guarantees regarding a wide class of CV schemes, namely those satisfying a balance condition, Assumption 2 below. We state and prove a generic upper bound on the error of the generalization risk estimate for stable algorithms. In the particular case where the validation size is fixed and small compared with the full sample our generic bound yields a control of the error which is comparable to the results in Celisse and Guedj 2016; Cornec 2017 for the l.p.o. case and in Bousquet and Elisseeff 2002 for the l.o.o.. It is also consistent with the findings of Shao 1993, 1997; Yang 2007 mentioned above which concern model selection. However, for the K-fold CV, the ratio between the validation and training sample sizes is fixed and the obtained upper bound is not satisfactory, in so far as it does not vanish as \(n \to \infty\).

Our main contributions are gathered in sections 4 to 6 and may be summarized as follows:

1. One may wonder whether the looseness of the bound for the specific case of the K-fold is just an artifact from our proof. We answer in the negative by deriving a lower bound for the K-fold (Section 4). The latter bound shows that under the uniform stability assumption alone, K-fold CV is inefficient in so far as it can fail in estimating the
generalization risk of a uniformly stable algorithm. In other terms one cannot construct a vanishing universal upper bound for the K-fold estimation error even though the stability property allows one to do so regarding the empirical risk itself.

2. We propose a corrected CV procedure which is well defined for any CV scheme. For this corrected CV scheme we prove a PAC generalization upper bound covering the general case of uniformly stable learners and any CV scheme satisfying a balance condition (Assumption 2). As a consequence the corrected version of the K-fold is shown to be efficient contrarily to the standard version. The corrected K-fold scheme has been investigated in Burman 1989; Arlot and Lerasle 2016 in the particular frameworks of linear regression and density estimation. Instead our upper bound covers the general case of uniformly stable learners and applies to most CV procedures. As an example of application, we show that the debiased K-fold permits to select a model within a finite collection in a risk consistent manner (Section 6), in other words, the excess risk of the selected model tends to 0 as \( n \to \infty \). Finally we demonstrate empirically (Section 7) the added value of the debiased K-fold compared with the standard one in terms of the test error of the selected model.

To sum up, in section 3 we generalize existing results from the algorithmic stability literature in order to provide some context about the lack of guarantee regarding the standard Kfold in a self-contained manner and to motivate the rest of this work. The novelty of this paper mainly resides in Contribution 1 (lower bound for the K-fold) and Contribution 2 (debiased version) listed above. Indeed we believe that the generic lower bound and the debiased scheme that we promote are the first of their kind for the K-fold in a general stability framework.

2 Background, notations and working assumptions

2.1 Notations

We place ourselves in the following general learning setting. One receives a collection of independent and identically distributed random vectors \( D = (O_1, \ldots, O_n) \) lying in a sample space \( Z \), with common distribution \( P \). For any \( n \in \mathbb{N} \), let \([n]\) denote the set of integers \( \{1, 2, \ldots, n\} \). Consider a class of predictors \( \mathcal{G} \) and a loss function \( \ell : \mathcal{G} \times Z \to \mathbb{R} \), so that \( \ell(g, O) \) be the error of \( g \) on the observation \( O \in Z \). As an example in the supervised learning setting \( Z = \mathcal{X} \times \mathcal{Y} \), \( g \) is a mapping \( \mathcal{X} \to \mathcal{Y} \) and for \( o = (x, y) \) the loss function writes as \( \ell(g, o) = \ell(g(x), y) \). However our results are not limited to the supervised setting. Given a subsample \( D_T = \{O_i \mid i \in T\} \) indexed by \( T \subset [n] \) and an algorithm (or learning rule) \( \mathcal{A} \), we denote by \( \mathcal{A}(T) \in \mathcal{G} \) the predictor obtained by training \( \mathcal{A} \) on \( D_T \). The generalization risk of the predictor \( \mathcal{A}(T) \) is then

\[
R[\mathcal{A}(T)] = \mathbb{E} [\ell(\mathcal{A}(T), O) \mid D_T],
\]

where \( O \) is independent from \( D_T \). Notice that the randomness in the latter expectation stems from the novel observation \( O \) only while the trained algorithm \( \mathcal{A}(T) \) is fixed. The quantity of interest here is the generalization risk of the learning rule trained on the full dataset, \( R[\mathcal{A}([n])] \). The hold-out estimate of the latter involves a validation index set \( V \) disjoint from
and writes as

\[
\hat{R}[A(T), V] = \frac{1}{n_V} \sum_{i \in V} \ell(A(T), O_i),
\]

where \( n_V = \text{card}(V) \).

Given a family of validation sets in \([n]\), \( V_{1:K} = (V_j)_{j=1,\ldots,K} \), the CV estimator of the generalization risk of \( A([n]) \) is

\[
\hat{R}_{CV}[A, V_{1:K}] = \frac{1}{K} \sum_{j=1}^{K} \hat{R}[A(T_j), V_j],
\]

where \( T_j = [n] \setminus V_j \). For clarity reasons, we suppose further that \( n \) is divisible by \( K \) so that \( n/K \) is an integer. This condition guarantees, in the case of \( K \)-fold cross validation, that all validation sets have the same cardinal \( n_V = n/K \).

**Remark 2.1.** While the K-fold procedure is associated to a constant value of \( K \) typically ranging between 2 and 10 regardless of the sample size \( n \), in our generic upper bounds (Theorem 3.1) we allow the number of folds \( K \) to grow with \( n \). Allowing this is important in order to include other popular cross-validation strategies such as the leave-one-out (l.o.o.) where the validation sets \( V_i \) are singletons, that is \( K = n \).

**Remark 2.2.** We further suppose that given a subsample \( \mathcal{D}_T \), the output of the algorithm \( A(T) \) is deterministic. In other words, running twice the algorithm on the same subsample produces the same result. In most examples, this assumption concerns the optimization routine that is employed to run the algorithm. We thereby neglect the randomness brought by the optimization routine. This assumption can be removed at the price of additional notational burden. For the sake of readability we adopt this deterministic assumption in the main paper and show how to relax it in the supplementary material (Section D), in order to cover the case of random algorithms such as SGD or neural networks.

### 2.2 Algorithmic Stability

An algorithm \( A \) is called stable if removing a training point \( O_i \) from \( \mathcal{D}_T \) (\( i \in T \)) or replacing \( O_i \) with an independent observation \( O' \) drawn from the same distribution does not change much the risk of the output. Formally, for \( i \in T \subset [n] \) as above, let \( T^\setminus i = T \setminus \{i\} \), so that \( A(T^\setminus i) \) is the output of \( A \) trained on \( \mathcal{D}_T \setminus \{O_i\} \). Denote similarly \( A(T^i) \) the output of \( A \) trained on \( \mathcal{D}_T \setminus \{O_i\} \cup \{O'\} \).

The notion of Hypothesis stability was first introduced in Devroye and Wagner 1979 to derive non asymptotic guarantees for the leave-one-out estimate. In this paper, we consider instead uniform stability, an assumption used in Bousquet and Elisseeff 2002 to derive probability upper bounds for the training error and the l.o.o. estimate. Equipped with the above notations, Uniform stability also called leave-one-out stability can be defined as follows.

**Definition 2.1.** An algorithm \( A \) is said to be \((\beta_t)_{1 \leq t \leq n}\)-uniformly stable with respect to a loss function \( \ell \) if, for any \( T \subset [n] \), \( i \in T \) it holds with \( P \)-probability one that

\[
\left| \ell(A(T), O) - \ell(A(T^\setminus i), O) \right| \leq \beta_{n_T}.
\]

(2.2)
If an algorithm is uniformly stable, then it is also change-one stable. A related, weaker notion of stability is change-one-stability. The formal definition parallels Definition 2.1, the only difference being, as the name suggests, that $T \setminus i$ is replaced with $T_i$. The link between these two notions is summarized by the following fact.

**Fact 2.1.** If an algorithm $A$ is $(\beta_t)_{1 \leq t \leq n}$ uniformly stable with respect to a loss function $\ell$ then, $A$ is $(2\beta_t)_{1 \leq t \leq n}$ change-one stable. In other words, for any $T \subset [n]$, $i \in T$ and $o, o' \in \mathbb{Z}_0 \subset \mathbb{Z}$ where $P(\mathbb{Z}_0) = 1$, the following holds,

$$|\ell(A(T), o) - \ell(A(T_i), o')| \leq 2\beta n T.$$ 

We provide the (simple) proof of this result in the appendix for completeness.

**Remark 2.3.** In the literature, uniform stability can refer to either leave-one-out (Bousquet and Elisseeff 2002) or change-one stability (Hardt et al. 2016). In fact, many popular algorithms (SVM, SGD, Least square regression) verify both hypothesis. However, this breaks up in some special cases, for example, as pointed out in Kutin and Niyogi 2002, if the performance of a learning rule $A$ depends on the parity of $n$ then $A$ can verify the change one hypothesis without verifying leave-one-out hypothesis.

The following simple fact concerns the effect of removing $n'$ training points on uniformly stable algorithms.

**Fact 2.2.** Let $A$ be a decision rule which is $(\beta_t)_{1 \leq t \leq n}$ uniformly stable, additionally suppose that the sequence $(\beta_t)_{1 \leq t \leq n}$ is decreasing, then for any $T \subset [n]$, with $P$-probability one, one has,

$$|\ell(A([n]), o) - \ell(A(T), O)| \leq (n - n'r)\beta n T.$$

Note that the monotonicity assumption regarding $(\beta_t)_{1 \leq t \leq n}$ is natural. Indeed, increasing the sample size has an overall stabilizing effect on learning algorithms.

**Remark 2.4.** Facts 2.1 and 2.2 play a key role in our proofs. Namely we use Fact 2.2 to control the bias of the CV risk estimate and Fact 2.1 to derive a probability upper bound on its deviations via McDiarmid’s inequality.

### 2.3 Working Assumptions

Throughout this paper we work under the following uniform stability assumption.

**Assumption 1 (Stable algorithm).** The algorithm $A$ is $(\beta_t)_{1 \leq t \leq n}$ uniformly stable with respect to a cost function $\ell$ that satisfies with probability one,

$$\forall T \subset [n], 0 \leq \ell(A(T), O) \leq L.$$

Following the line of Bousquet and Elisseeff 2002 and Hardt et al. 2016, we shall consider uniformly stable rules with stability parameter $\beta_n \leq \frac{\lambda}{n}$ for some $\lambda > 0$.

**Discussion.** Assumption 1 is indeed verified for many standard algorithms. In particular $\beta_n = O(\frac{1}{\sqrt{n}})$ for SVM/least square regression with the usual mean squared error, SVM classifier with the soft margin loss (Bousquet and Elisseeff 2002), SGD with convex and non convex...
losses (Hardt et al. 2016) and stochastic gradient methods like RGD (randomized coordinate descent), SVRG (stochastic variance reduced gradient method) with loss functions verifying the Polyak-Lojasiewicz condition (Charles and Papailiopoulos 2018).

We also need the sequence of validation and training sets to satisfy a certain balance condition which is expressed below.

**Assumption 2** (Validation sets balance condition). The validation sets $V_1, V_2, \ldots V_K$ satisfy

$$\text{card}(V_j) = n_V \quad \forall j \in [1, K],$$

for some $n_V \in [1, n]$. Moreover it holds that

$$\frac{1}{K} \sum_{j=1}^{K} \mathbb{1}\{l \in V_j\} = \frac{n_V}{n} \quad \forall l \in [n].$$

Because $T_j = [n] \setminus V_j$, if (2.4) holds, then the training sets $T_j$ verify a similar equation, that is,

$$\frac{1}{K} \sum_{j=1}^{K} \mathbb{1}\{l \in T_j\} = \frac{n_T}{n} \quad \forall l \in [n].$$

In Lemma A.1 in the appendix we show that Assumption 2 holds true both for the K-fold and the l.p.o.

### 3 Upper bounds for CV risk estimation

Our first result Theorem 3.1 is a generic upper bound on the error of the generalization risk estimate for stable algorithms satisfying Assumption 1 with general CV procedures verifying Assumption 2. Thus our conditions regarding the CV scheme are weaker than in Celisse and Guedj 2016; Cornec 2017 where only the l.p.o. error is considered, although our stability assumptions are stronger, since uniform stability is required here instead of $L^q$-stability as discussed in the introduction.

**Theorem 3.1.** Consider a stable learning algorithm $A$ satisfying Assumption 1 with $\beta_t \leq \frac{\lambda}{2}$, for some $\lambda > 0$. Then, for all CV schemes verifying Assumption 2, we have with probability $1 - 2\delta$,

$$\left| \hat{\mathcal{R}}_{CV} [A, V_{1:K}] - \mathcal{R} [A([n])] \right| \leq \lambda \frac{n_V}{n_T} + (4\lambda + L) \sqrt{\frac{\log(1/\delta)}{2n}}.$$

Where $L$ is the upper bound on the cost function $\ell$ from Assumption 1.

**Sketch of proof.** Define the average risk of the family $(A(D_{T_j}))_{1 \leq j \leq K}$

$$\mathcal{R}_{CV} [A, V_{1:K}] = \frac{1}{K} \sum_{j=1}^{K} \mathcal{R} [A(T_j)].$$


then write the following decomposition

\[ \hat{R}_{CV} [A, V_{1:K}] - R [A([n])] = D_{CV} + \text{Bias}, \] (3.2)

with

\[ D_{CV} = \hat{R}_{CV} [A, V_{1:K}] - R_{CV} [A, V_{1:K}], \] (3.3)

\[ \text{Bias} = R_{CV} [A, V_{1:K}] - R [A([n])]. \] (3.4)

The proof consists in bounding each term of the above decomposition independently. The term \( D_{CV} \) measures the deviations of \( \hat{R}_{CV} \) from its mean and it can be controlled using McDiarmid’s inequality (Proposition A.1). The second term \( \text{Bias} \) is controlled using Fact 2.2. The detailed proof is deferred to the appendix.

Discussion. Applying Theorem 3.1 to the leave-one-out procedure (\( n_V = 1 \)) yields the same bound as in Theorem 12 from Bousquet and Elisseeff 2002. Our result is more general in that it applies to a wider class of CV schemes, including l.o.o., l.p.o., K-fold and the repeated K-fold. A second novelty in Theorem 3.1 is its level of generality regarding the class of algorithms compared to existing works investigating model selection in more restrictive frameworks such as regression Shao 1997; Yang 2007, and density estimation Arlot and Lerasle 2016.

In the remainder of this section, we apply Theorem 3.1 to control the estimation error of some standard CV procedures, namely l.p.o. and K-fold CV. The two next corollaries are immediate consequences of Theorem 3.1 and Lemma A.1 ensuring that both K-fold and l.p.o. satisfy Assumption 2.

**Corollary 3.1** (l.p.o. upper bound). Suppose that Assumption 1 holds with \( \beta_t \leq \frac{\lambda}{T} \), for some \( \lambda > 0 \). Then, we have, with probability \( 1 - 2\delta \),

\[ \left| \hat{R}_{lpo} [A, V_{1:K}] - R [A([n])] \right| \leq \frac{\lambda p}{n - p} + (4\lambda + L) \sqrt{\frac{\log(1/\delta)}{2n}}, \]

where \( \hat{R}_{lpo} \) is the l.p.o. estimate, and \( L \) is the upper bound of the cost function.

**Corollary 3.2** (K-fold upper bound). Suppose that Assumption 1 holds with \( \beta_t \leq \frac{\lambda}{T} \), for some \( \lambda > 0 \). Then, we have, with probability \( 1 - 2\delta \),

\[ \left| \hat{R}_{Kfold} [A, V_{1:K}] - R [A([n])] \right| \leq \frac{\lambda}{K - 1} + (4\lambda + L) \sqrt{\frac{\log(1/\delta)}{2n}}, \]

where \( \hat{R}_{Kfold} \) is the K-fold estimate, and \( L \) is the upper bound of the cost function.

In the above corollary the upper bound is not consistent in the sense that it does not tend to 0 as \( n \to \infty \). In the next section we confirm this negative result with a lower bound regarding the deviations of the K-fold risk estimate.
4 Lower bound for the K-fold error under algorithmic stability

The next result confirms that uniform stability is not sufficient to ensure consistency of the K-fold CV risk estimate. The counter-example that we build to prove a lower bound is formulated in a regression framework.

**Theorem 4.1** (Non vanishing lower bound on the K-fold error). Consider the regression problem for a random pair \(O = (X, Y) \in \mathcal{Z} = \mathcal{X} \times \mathbb{R}\) with distribution \(P\), and loss function \(\ell(g, o) = |g(x) - y|\). Let \(n \geq 2, M \geq \log(n)\) and \(0 \leq \lambda \leq \frac{1}{M}\). There exists an algorithm \(A\) verifying Assumption 1 with \(\beta_t = 3\lambda/t\), and \(L = (M + 1)^2\), and a distribution \(P\) such that

\[
E\left[\left|\hat{R}_{\text{Kfold}}[A, V_{1:K}] - R[A([n])]\right|\right] \geq \frac{\lambda}{2K^2} - \frac{2\lambda}{n}.
\]

**Sketch of proof.** Let \(\mathcal{X}\) be a finite grid of size \(n\),

\[
\mathcal{X} = \{x_1, \ldots, x_n\}
\]

with \(x_m = MS_m, S_m = \sum_{j=1}^{m} (1/j)\). Let \(P\) be the uniform distribution over the finite set \(\{(x, f_n(x)) : x \in \mathcal{X}\}\), where \(f_n(x_m) = x_m + \sigma_m \epsilon\) where \(0 < \epsilon < \lambda n\) is a fixed constant and

\[
\sigma_m = \begin{cases} 
1 & \text{if } m \leq \lfloor n/2 \rfloor \\
-1 & \text{if } m > \lfloor n/2 \rfloor.
\end{cases}
\]

In this context, the target \(y_m = f_n(x_m)\) for some \(m \leq n\) is the sum of a signal term \(x_m = MS_m\) and a noise term \(\sigma_m \epsilon\), the sign of which depends deterministically on the position of \(X = x_m\) with respect to the median \(x_{\lfloor n/2 \rfloor}\). Draw a dataset

\[
\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}
\]

made of independent observations from \(P\). For a training sequence indexed by \(T \subset [n]\), for a given \(x_m = MS_m \in \mathcal{X}\), define the learning rule

\[
A(T)(x_m) = \lambda S_{\min(m, n_T)} + \epsilon \text{sign}(\text{med}(\mathcal{D}_T) - x_m).
\]

The idea behind the predictor \(A(T)\) is as follows: \(\lambda S_{\min(m, n_T)}\) mimics the signal while the term \(\text{sign}(\text{med}(\mathcal{D}_T) - x_m)\) tries to capture the sign \(\sigma_m\) of the noise term \(\sigma_m \epsilon\). This rule is thus better than a random guess. The remainder of the proof proceeds according to the following main steps

1. Show that \(\ell\) is \((M + 1)^2\)-bounded.

2. Verify the uniform stability assumption \(i.e.,\) for any training set \(T \subset [n]\), for any index \(j \in T\), with probability one,

\[
|\ell(A(T), O) - \ell(A(T^\cup j), O)| \leq \frac{3\lambda}{n_T}.
\]
3. Compute the true risks $R[A(T)]$ and $R[A([n])]$.

4. Deduce that $R[A(T)] - R[A([n])] \geq \frac{1}{2K^2} - \frac{2\lambda}{n}$.

The result follows by an application of the tower rule for conditional expectations. The technical details are gathered in the appendix (Section C.3).

**Discussion.** Theorem 4.1 reveals the suboptimality of K-fold CV in the general stability framework for risk estimation. For the purpose of model selection, which is arguably a harder problem, existing works have shown the suboptimality of K-fold CV. For example, in a linear regression framework, Yang 2007 (See also (Yang 2006) for classification problems) has shown that the usual K-fold procedure may not select the best model with probability going to one. For efficient model selection, where the performance is measured in terms of generalization risk of the selected model, Arlot 2008 shows (See Theorem 1 in the latter reference) that K-fold CV can be suboptimal, i.e. an example is provided where the risk ratio between the selected model and the optimal one is uniformly greater (for all $n$) than $1 + \kappa$ for some $\kappa > 0$. In Theorem 4.1 of the present paper we show a stronger result, in so far as we consider the easier task of risk estimation, and we show that K-fold CV with fixed $K$ does not enjoy sanity-check guarantees because for any $n$, there exists a regression problem where the error is at least $\lambda/(2K^2)$.

In the next section, we show that adding correction terms (Burman 1989) to K-fold CV addresses the inconsistency issues underlined by Theorem 4.1. The resulting CV scheme enjoys both the computational efficiency of the K-fold (compared with the l.p.o.), and finite sample guarantees comparable to those of the l.p.o. in view of the upper bound stated in Theorem 5.1.

5 **Bias corrected K-fold with stable learners**

A key ingredient of the lack of guarantee regarding the K-fold risk estimate is its bias for finite sample sizes, an issue pointed out by Burman 1989 who proposes a corrected version of the standard K-fold with a reduced bias. In the present work we follow in the footsteps of Burman 1989 and consider the same corrected CV estimate of the generalization risk

$$\hat{R}_{CV}^{corr} [A, V_{1:K}] = \hat{R}_{CV} [A, V_{1:K}] + \hat{R} [A([n])], [n]] - \frac{1}{K} \sum_{j=1}^{K} \hat{R} [A(T), [n]].$$

The correcting term (second line in the above display) is the difference of the empirical risks between $A([n])$ and $A(T)$. In Burman 1989 the analysis is carried out in an asymptotic framework and focuses on the asymptotic bias and variance of the estimator for different CV schemes. The results are obtained under differentiability assumptions regarding the algorithm $A$. In contrast, we conduct here a non asymptotic analysis relying on algorithmic stability alone. Our results summarized in the next theorem are valid for any CV scheme (including the K-fold) satisfying the balance condition Assumption 2.
Theorem 5.1. Suppose that Assumption 1 holds with \( \beta_n \leq \frac{1}{n} \), for some \( \lambda > 0 \). Then, for all CV schemes verifying Assumption 2, we have, with probability \( 1 - 6\delta \),

\[
\left| \hat{R}_{\text{CV}}^{\text{corr}}[A, V_{1:K}] - \mathcal{R}[A([n])] \right| \leq 2\lambda \left( \frac{1}{n} + \frac{1}{n_T} \right) + 3(4\lambda + L) \sqrt{\frac{\log(1/\delta)}{2n}}.
\]

Sketch of proof. By simple algebra write the corrected CV estimator as

\[
\hat{R}_{\text{CV}}^{\text{corr}}[A, V_{1:K}] = \hat{R}[A([n]), [n]] + \frac{n_T}{nK} \sum_{j=1}^{K} \left( \hat{R}[A(T_j), V_j] - \hat{R}[A(T_j), T_j] \right).
\]

From this, deduce the following error decomposition

\[
\hat{R}_{\text{CV}}^{\text{corr}}[A, V_{1:K}] - \mathcal{R}[A([n])] = D_{A[n]} + \frac{n_T}{n} (D_{\text{CV}} - D_{A[T_1,K]}),
\]

where \( D_{\text{CV}} \) is defined in (3.3) and

\[
D_{A[n]} = \hat{R}[A([n]), [n]] - \mathcal{R}[A[n]],
\]

\[
D_{A[T_1,K]} = \frac{1}{K} \sum_{j=1}^{K} \left( \hat{R}[A(T_j), T_j] - \mathcal{R}[A(T_j)] \right).
\]

Notice the absence of a bias term in the above display, contrarily to the error decomposition (3.2) for the standard CV estimate in the proof of Theorem 3.1. The remaining technical arguments for bounding each term of the decomposition above are gathered in the supplement. Namely, using McDiarmid’s inequality (Proposition A.1), we derive concentration bound both for \( D_{\text{CV}} \) as stated in Lemma B.1 and for \( D_{A[T_1,K]} \) as given in Lemma B.2. Finally the deviations of the empirical risk \( D_{A[n]} \) are controlled using Remark B.1, a consequence of Lemma B.2, in the supplement, which yields a bound similar in spirit to Theorem 12 in Bousquet and Elisseeff 2002.

Theorem 5.1 yields immediately a consistent upper bound for the K-fold CV error. For the proof it suffices to notice that \( n_T = \frac{K-1}{K} n \) for the K-fold scheme and to use that \( (2K-1)/(K-1) \leq 3 \) whenever \( K \geq 2 \).

Corollary 5.1. Suppose that Assumption 1 holds with \( \beta_n \leq \frac{1}{n} \), for some \( \lambda > 0 \). Then, the error of the corrected K-fold CV (with \( K \geq 2 \)) estimate of the generalization risk satisfies with probability at least \( 1 - 6\delta \)

\[
\left| \hat{R}_{\text{K-fold}}^{\text{corr}}[A, V_{1:K}] - \mathcal{R}[A([n])] \right| \leq \frac{6\lambda}{n} + 3(4\lambda + L) \sqrt{\frac{\log(1/\delta)}{2n}}.
\]

Discussion. Corollary 5.1 confirms the consistency of the bias corrected K-fold for risk estimation purpose with uniformly stable learners. Existing works in this direction (Burman 1989; Arlot and Lerasle 2016) are limited to specific tasks, namely respectively linear regression and density estimation. Thus our results show that indeed correcting the K-fold ensures its consistency for estimating the generalization risk of any uniformly stable learner like SGD, SVM and neural networks with a simple architecture.
In the next section we turn to the problem of model selection which is a different and arguably harder problem than risk estimation if the goal is to select the best model mainly because different models may have comparable performance. However if one aims only at selecting a model for which the generalization risk is close to that of the optimal one, lack of identifiability is not necessarily an issue anymore. This is precisely the approach we take here.

6 Application to model selection

It is a known fact that cross-validation is in general sub-optimal for model selection for model identification purpose, i.e. when the goal is to identify the best model. A major reason for this is that \( \hat{R}_{CV} [A, V_{i:K}] \) is a biased estimate of \( R[A([n])] \). An alternative and more attainable goal is efficient model selection (see e.g. Arlot and Lerasle 2016 and the references therein) aiming at selecting a model for which the generalization risk of the learnt predictor is close to the smallest possible risk.

We start off with a brief description of the model selection setting. Given a family of models (or algorithms) \( A^{(m)} \) indexed by \( m \in \mathcal{M} \) and a dataset \( D \) of size \( n \), an optimal model \( A^{(m^*)} \) called an oracle is any model such that

\[
A^{(m^*)} \in \arg \min_{m \in \mathcal{M}} R[A^{(m)}([n])]. \tag{6.1}
\]

Since the true risk is unknown, an empirical criterion must be used instead to select an efficient model. One of the most popular tools for model selection is K-fold CV. However, as discussed earlier, the latter procedure can be inconsistent. To tackle this issue, we propose to use the corrected K-fold and select a model \( A^{(\hat{m})} \) such that

\[
A^{(\hat{m})} \in \arg \min_{m \in \mathcal{M}} \hat{R}_{Kfold}^{corr} [A^{(m)}, V_{1:K}]. \tag{6.2}
\]

We obtain in Theorem 6.1 an upper bound in probability for the excess risk \( R[A^{(\hat{m})}([n])] - R[A^{(m^*)}([n])] \) in the case where the family of models \( \mathcal{M} \) is finite. Since this upper bound converges to 0 as \( n \to \infty \), our result ensures in particular the consistency of the selection procedure.

**Theorem 6.1.** Let \( (A^{(m)})_{m \in \mathcal{M}} \) be a family of algorithms where each learner \( A^{(m)} \) is \((\beta_{m,t})_{1 \leq t \leq n}\) uniformly stable with respect to a loss function \( 0 \leq \ell(g, O) \leq L \). Additionally, assume that,

\[
\forall m \in \mathcal{M} ; \beta_{m,t} \leq \frac{M}{t},
\]

for some \( M > 0 \). Then one has, with probability at least \( 1 - 6\delta \),

\[
R[A^{(\hat{m})}([n])] - R[A^{(m^*)}([n])] \leq \frac{12M}{n} + 6M + 6L \sqrt{\frac{\log(|\mathcal{M}|/\delta)}{n}}.
\]

**Proof.** The proof is deferred to the Appendix. \( \square \)
Discussion (bounded stability parameters $\beta_{m,t}$’s). The assumption $\beta_{m,t} \leq \frac{M}{t}$ for all $m$ is indeed verified in many applications. For example, in regularized SVM, where each learner $A^{(m)}$ is trained using a regularization parameter $\gamma_m$, Bousquet and Elisseeff 2002 show that $\beta_{m,t} = \frac{1}{t^2} \sqrt{\frac{C}{\gamma_m}}$ where $C$ is a positive constant. Thus if one performs a grid search for $\gamma_m$ in a grid $[a,b]$ with $a > 0$, then $\beta_{m,t} \leq \frac{1}{t} \sqrt{\frac{C}{a}}$ for any $\gamma_m \in [a,b]$. In other words, since the search space is generally bounded, the assumption about the boundedness of the $\beta_{m,t}$’s is not too restrictive in practice.

7 Experimental results

The aim of our experiments is to illustrate empirically the added value of the corrected K-fold compared with the standard one in terms of efficiency in model selection. In other words we perform model selection with the K-fold and the corrected version that we promote and we compare the generalization risks of the selected trained models.

7.1 Experimental Setting

We choose as a family of models $\mathcal{M}$ a family of SVM regressors and classifiers trained with a regularization parameter $\gamma_m$ ranging in a finite grid in an interval $[a,b]$. Namely we set $[a,b] = [0.1, 100]$, and the grid is constructed with a constant step size equal to $\Delta = 0.1$, so that

$$(\gamma_m)_{m \in \mathcal{M}} = \{a + j\Delta \mid 0 \leq j < 1000\}.$$ 

In this SVM framework,

$$A^{(m)}(T) = \arg\min_{f \in \mathcal{F}} \frac{1}{n_T} \sum_{i \in T} \ell(f, O_i) + \gamma_m \|f\|_k$$

where $\mathcal{F}$ is a reproducing kernel Hilbert space with kernel $k$. We use the implementation provided by the python library scikit-learn. The kernel $k$ is chosen here as the sigmoid kernel $\tanh(\tau \langle x, \rangle)$. Following standard practice we set $\tau = \frac{1}{d}$, where $d$ is the dimension of the dataset. The assumptions of Theorem 6.1 are thus satisfied, as pointed out in the discussion following the theorem’s statement. We use the quadratic loss for regression problems and the hinge loss $\ell(g, (x, y)) = (1 - yg(x))_+$ for classification, where $(f(x))_+ = \max(0, f(x))$. Since the training datasets are bounded, we may consider that both these losses as bounded as well. For both these losses the algorithm $A^{(m)}$ is $\frac{1}{n}$ uniformly stable (see Bousquet and Elisseeff 2002 for further details).

7.2 Datasets

Eight reference datasets from UCI $^1$ are considered: four classification datasets and four regression datasets listed below.

$^1$https://archive.ics.uci.edu
Regression datasets

- *Real estate valuation* (REV, 414 house price of unit area with 5 covariates);
- *QSAR fish toxicity* (906 toxic chemical concentration with 6 attributes);
- *Energy efficiency* (EE, 768 heating loads with 8 features);
- *Concrete Compressive Strength* (CS, 1030 measure of the compressive strength with 8 attributes).

Classification datasets

- *Ionosphere dataset* (IO, 351 radar returns with 34 attributes),
- *Raisin dataset* (RS, 900 Keciman/Besni raisin with 7 attributes),
- *Audit risk dataset* (AR, 777 firm evaluation (fraudulent/non fraudulent) with 18 risk factors) and
- *QSAR bio degradation Data Set* (BIODEG, 1055 chemicals categorization with 12 descriptive features).

For each dataset one third of the data are removed ($S$) and reserved for testing, *i.e.* for evaluating the generalization risk of the model selected using the remaining two thirds ($D$).

Let $\hat{m}_{Kf}$ (resp. $\hat{m}_{Kf-corr}$) denote the model selected using K-fold CV (resp. corrected K-fold CV) on the train set $D$. In other words

$$A(\hat{m}_{Kf-corr}) = \arg \min_{m \in M} \hat{R}_{Kfold}^{corr} \left[ A(m), V_{1:K} \right],$$

$$A(\hat{m}_{Kf}) = \arg \min_{m \in M} \hat{R}_{Kfold} \left[ A(m), V_{1:K} \right].$$

In the end, in line with Section 6, the performance of both models are compared in terms of generalization risk using the empirical risk on the test set $S$,

$$\hat{R} \left[ A_D(\hat{m}), S \right] = \frac{1}{n_S} \sum_{O_i \in S} l \left( A_D^{(\hat{m})}(i), O_i \right). \quad (7.1)$$

### 7.3 Results

Tables 1 and 2 gather the results obtained respectively with the regression and classification datasets, for different numbers of folds $K$ varying between 2 and 5. In all cases, the model selected by the bias corrected K-fold has a lower generalization risk than the one selected by the standard K-fold. As expected, the standard K-fold procedure behaves generally better with $K = 5$ than with $K = 2$. Indeed larger values of $K$ decrease the bias of the K-fold CV. The benefit of the bias correction is thus all the more important for small values of $K$.

### 8 Conclusion

This paper demonstrates the limitations of the standard K-fold procedure for risk estimation via a lower bound on its error with a uniformly stable learner. We show that the corrected version of the K-fold for uniformly stable algorithms does not suffer the same drawbacks through a sanity-check upper bound and leverage this result to obtain guarantees regarding efficient model selection. This paves the way towards two possible research directions. First, it would be valuable to relax our uniform stability assumption in order to cover a still wider class of algorithms such as k-nearest-neighbors (Devroye and Wagner 1979), Adaboost (Freund and Schapire 1997) and Lasso regression (Celisse and Guedj 2016). A second promising avenue is to consider an extension of the K-fold penalization proposed by Arlot and Lerasle 2016 to the class of stable learners.
Table 1: Regression mean squared errors for the K-fold and the bias corrected K-fold on various data sets.

| Dataset  | K-fold | Bias corrected K-fold |
|----------|--------|-----------------------|
| REV; K=3 | 74.198 | 68.958                |
| REV; K=4 | 74.189 | 68.958                |
| REV; K=5 | 73.359 | 68.958                |
| EE; K=3  | 15.501 | 14.405                |
| EE; K=4  | 15.825 | 14.35                 |
| EE; K=5  | 14.73  | 14.298                |
| QSAR; K=3| 1.183  | 1.035                 |
| QSAR; K=4| 1.112  | 1.035                 |
| QSAR; K=5| 1.112  | 1.035                 |
| CS; K=3  | 146.881| 126.492               |
| CS; K=4  | 144.195| 124.205               |
| CS; K=5  | 137.06 | 123.641               |

Table 2: Hinge losses for the K-fold and the bias corrected K-fold on various data sets.

| Dataset  | K-fold | Bias corrected K-fold |
|----------|--------|-----------------------|
| RS; K=3  | 0.47   | 0.419                 |
| RS; K=4  | 0.42   | 0.418                 |
| RS; K=5  | 0.42   | 0.419                 |
| IO; K=3  | 0.454  | 0.414                 |
| IO; K=4  | 0.447  | 0.425                 |
| IO; K=5  | 0.477  | 0.464                 |
| BIODEG; K=3| 0.361 | 0.357                 |
| BIODEG; K=4| 0.363 | 0.357                 |
| BIODEG; K=5| 0.381 | 0.357                 |
| AR; K=3  | 0.112  | 0.109                 |
| AR; K=4  | 0.108  | 0.105                 |
| AR; K=5  | 0.107  | 0.106                 |

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A Main tools

First we recall McDiarmid’s inequality (Theorem 3.1 in (McDiarmid 1998)).

**Proposition A.1** (McDiarmid’s inequality). Let $Z = f(D)$ for some measurable function $f$ and define

$$
\Delta_l(D, O') = f(D) - f(D^l),
$$

where $D^l$ is obtained by replacing the $l$’th element of $D$ by a sample $O' \in Z$. In addition, suppose that

$$
\forall l \in [n], \sup_{D \in Z} \sup_{O' \in Z} |\Delta_l(D, O')| \leq c_l.
$$

Then for any $t \geq 0$,

$$
P(Z - \mathbb{E}(Z) \geq t) \leq \exp \left( -\frac{2t^2}{\sum_{l=1}^{n} c_l^2} \right).
$$

The following lemma guarantees that Assumption 2 is verified for standard CV-procedures.

**Lemma A.1.** For leave-one-out, leave-$p$-out, and $K$-fold procedures, the training samples $T_{1:K}$ and validation samples $V_{1:K}$ satisfies assumption 2 i.e.

$$
\frac{1}{K} \sum_{j=1}^{K} \frac{1 \{ l \in T_j \}}{n_T} = \frac{1}{K} \sum_{j=1}^{K} \frac{1 \{ l \in V_j \}}{n_V} = \frac{1}{n} \forall l \in [1, n].
$$

**Proof.** Since the leave-one-out can be seen as a special case of $K$-fold with $K = n$, it suffices to treat only the case of the leave-$p$-out and the $K$-fold.

**$K$-Fold.** For this procedure, the validation sets verify the following property

$$
\bigcup_{j=1}^{K} V_j = \llbracket 1, n \rrbracket \text{ and } V_j \bigcap V_k = \emptyset, \forall j \neq k \in [1, K]. \quad (A.1)
$$

Under the hypothesis that $\text{card}(V_j) = n_V$ for all the validation sets, (A.1) implies that

$$
n = \sum_{j=1}^{K} \text{card}(V_j) = Kn_V. \quad (A.2)
$$

Furthermore, under (A.1), an index $l \in [1, n]$ belongs to a unique validation test $V_j'$ and to all the train sets $T_j = V_j'$ with $j \neq j'$. Hence, we have

$$
\begin{cases}
\sum_{j=1}^{K} 1 \{ l \in T_j \} = K - 1, \\
\sum_{j=1}^{K} 1 \{ l \in V_j \} = 1.
\end{cases}
$$

Using (A.1) and the fact that $n_T = n - n_V = (K - 1)n_V$ yields the desired result.
Leave-$p$-out. In the leave-$p$-out procedure, the validation sets are all the subsamples of $\mathcal{D}_n$ with $\text{card}(V_j) = p$, thus we have $K = \binom{n}{p}$. On the other hand, an index $l \in [1, n]$ belongs to $\binom{n-1}{p-1}$ validation sets. In fact, creating a $V_j$ such as $l \in V_j$ is equivalent to first picking $l$ and then choosing $m - 1$ element from $[1, n] \setminus \{l\}$. Hence we have

$$\sum_{j=1}^{K} \mathbb{1}\{l \in V_j\} = \binom{n-1}{p-1}, \forall l \in [1, n].$$

Recall that $n\binom{n-1}{p-1} = p\binom{n}{p}$ which yields

$$\frac{1}{Kn_v} \sum_{j=1}^{K} \mathbb{1}\{l \in V_j\} = \frac{1}{p\binom{n}{p}} \sum_{j=1}^{K} \mathbb{1}\{l \in V_j\} = 1/n.$$ 

Similar arguments can be used for the sequence $T_{1:K}$, and the proof is complete.

\[ \square \]

B Intermediate results

First we provide a concentration bound for $D_{CV}$ which has been defined in (3.3) as

$$D_{CV} = \hat{R}_{CV} \{ \mathcal{A}, V_{1:K} \} - R_{CV} \{ \mathcal{A}, V_{1:K} \}.$$ 

Lemma B.1. Suppose that Assumption 1 holds. Then, for all CV schemes verifying Assumption 2, we have

$$\mathbb{P}(|D_{CV}| \geq t) \leq \exp\left(\frac{-2t^2}{4\beta_{uv}nT + L}\right).$$

Proof. Let $O' \in \mathcal{X}$ be an independent copy of $O_1, O_2, \ldots, O_n$, for any $l \in [1, n]$ define

$$\Delta_l(D, O') = |D_{CV}(D) - D_{CV}(D^l)|,$$

where $D^l$ is obtained by replacing the $l$\textsuperscript{th} element of $D$ by $O'$. Now we derive an upper bound on $\mathbb{P}(|D_{CV}| \geq t)$ using Proposition A.1. Namely, we will bound the maximum deviation of $\Delta_l$ by $\Delta_l \leq \frac{4\beta_{uv}nT}{n} + \frac{L}{n}$. To do so, write

$$D_{CV} = \hat{R}_{CV} \{ \mathcal{A}, V_{1:K} \} - R_{CV} \{ \mathcal{A}, V_{1:K} \}$$

$$= \frac{1}{Kn_{val}} \sum_{j=1}^{K} \sum_{i \in V_j} \left( \ell(A(T_j), O_i) - \mathbb{E}_O[\ell(A(T_j), O) \mid D_{T_j}] \right)$$

$$= \frac{1}{Kn_{val}} \sum_{j=1}^{K} \sum_{i \in V_j} h(A(T_j), O_i),$$

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where the last is used to define \( h \). For a training set \( T_j \subset [n] \), let \( A(T_{j,l}) \) denote the algorithm \( A \) trained on the sequence \( D_{T_j,l} = \{O_i \in D^i \mid i \in T_j\} \). Note that, for all \( D_{T_j}, o \in \mathbb{Z}^{|\mathbb{E}|} \times \mathbb{Z} \) one has

\[
\ell(A(T_j), o) = \ell(A(T_{j,l}), o) \text{ if } l \notin T_j, \\
\ell(A(T_j), o) - \ell(A(T_{j,l}), o) \leq 2\beta_{nT} \text{ otherwise.} \tag{B.1}
\]

The first equation follows from the fact that \( D_{T_j} \), indeed, if the training set \( D_{T_j} \) doesn't contain the index \( l \) then changing the \( l \)th element of \( D \) won't affect \( D_{T_j} \). The second inequality is obtained using the uniform stability of \( A \) and fact 2.1. Furthermore, using Equation B.1 write

\[
\begin{align*}
\mathbb{E} \left[ \ell(A(T_j), O) \mid D_{T_j} \right] &= \mathbb{E} \left[ \ell(A(T_{j,l}), O) \mid D_{T_j,l} \right] \text{ if } l \notin T_j, \\
\mathbb{E} \left[ \ell(A(T_j), O) \mid D_{T_j} \right] - \mathbb{E} \left[ \ell(A(T_{j,l}), O) \mid D_{T_j,l} \right] &\leq 2\beta_{nT}, \text{ otherwise.} \tag{B.2}
\end{align*}
\]

Combining (B.2) and (B.1) gives

\[
\begin{align*}
&\left| \mathbb{1} \{l \in T_j\} (h(A(T_j), O_i) - h(A(T_{j,l}), O_i)) \right| \leq 4\beta_{nT}, \\
&\left| \mathbb{1} \{l \notin T_j\} (h(A(T_j), O_i) - h(A(T_{j,l}), O_i)) \right| \leq L \mathbb{1} \{i = l\}, \tag{B.3}
\end{align*}
\]

so that

\[
|\Delta_l(D, O')| \leq \frac{1}{Kn_{\text{val}}} \sum_{j=1}^{K} \sum_{i \in V_j} |h(A(T_j), O_i) - h(A(T_{j,l}), O_i)|
\]

(From the fact that \([n] \setminus T_j = V_j\) )

\[
= \frac{1}{Kn_{\text{val}}} \sum_{j=1}^{K} \sum_{i \in V_j} |h(A(T_j), O_i) - h(A(T_{j,l}), O_i)| (\mathbb{1} \{l \in T_j\} + \mathbb{1} \{l \in V_j\})
\]

(By Equation B.3) \leq \frac{4\beta_{nT}}{K} \sum_{j=1}^{K} \mathbb{1} \{l \in T_j\} + \frac{L}{n_{\text{val}}K} \sum_{j=1}^{K} \mathbb{1} \{l \in V_j\}

(By Assumption 2) \leq \frac{4\beta_{nT}n_T}{n} + \frac{L}{n}.

Using McDiarmid’s inequality (Proposition A.1) gives

\[\mathbb{P}(D_{CV} \geq t) \leq \exp \left( \frac{-2nt^2}{(4\beta_{nT}n_T + L)^2} \right).\]

Symmetrically, one has,

\[\mathbb{P}(D_{CV} \leq -t) \leq \exp \left( \frac{-2nt^2}{(4\beta_{nT}n_T + L)^2} \right).\]

Thus,

\[\mathbb{P}(|D_{CV}| \geq t) \leq 2 \exp \left( \frac{-2nt^2}{(4\beta_{nT}n_T + L)^2} \right),\]

which is the desired result. \( \square \)
In the next lemma we obtain a similar concentration bound for the term \(D_{A[T_1, K]}\) defined in Eq 5.4 as
\[
D_{A[T_1, K]} = \frac{1}{K} \sum_{j=1}^{K} \left( \hat{R} [A(T_j), T_j] - \mathcal{R} [A(T_j)] \right).
\]

**Lemma B.2.** Suppose that Assumption 1 holds. Then, for all CV schemes verifying Assumption 2, we have
\[
\mathbb{P}(|D_{A[T_1, K]}| \geq t + 2\beta_{n_T}) \leq \exp \left( \frac{-2nt^2}{(4\beta_{n_T}n_T + L)^2} \right),
\]
where \(L\) is the upper bound of the cost function defined in Assumption 1.

**Proof.** Though the proof bears resemblance with the one of Lemma B.1, we the full details for completeness. We use McDiarmid’s inequality with \(f(D) = D_{A[T_1, K]}\), that is,
\[
f(D) = \frac{1}{K} \sum_{j=1}^{K} \left( \hat{R} [A(T_j), T_j] - \mathcal{R} [A(T_j)] \right)
\] and
\[
f(D') = \frac{1}{K} \sum_{j=1}^{K} \left( \hat{R} [A(T_j, l), T_j, l] - \mathcal{R} [A(T_j, l)] \right).
\]

Since for \(l \notin T_j, T_j = T_{j,l}\), we find that
\[
|\Delta_l(D, O')| \leq \frac{1}{K n_T} \sum_{j=1}^{K} \mathbb{1} \{ l \in T_j \} \left( \hat{R} [A(T_j), T_j] - \hat{R} [A(T_{j,l}, T_{j,l})] + \mathcal{R} [A(T_{j,l})] - \mathcal{R} [A(T_j)] \right)
\]
\[
\leq \frac{1}{K n_T} \sum_{j=1}^{K} \mathbb{1} \{ l \in T_j \} \sum_{i \in T_j} |h(A(T_j), O_i) - h(A(T_{j,l}, O_i))|,
\]
with
\[
h(A(T), o) = \ell(A(T), o) - \mathbb{E}_O [\ell(A(T), O) \mid D_T] \quad \text{and} \quad (O_i)_{i=1,...,n} \quad \text{is the same as} \quad (O_i)_{i=1,...,n}
\]
except the \(l\)-th element, \(O_l\), which is replaced by \(O'\). Whenever \(l \in T_j\), it holds that
\[
|\ell(A(T_j), O_i) - \ell(A(T_{j,l}, O_i))| = |\ell(A(T_j), O_i) - \ell(A(T_j, l), O_i)| \mathbb{1} \{ i \neq l \} + |\ell(A(T_j, l), O_i) - \ell(A(T_{j,l}, O'_i))| \mathbb{1} \{ i = l \}
\]
\[
\leq 2\beta_{n_T} + L \mathbb{1} \{ i = l \},
\]
and that
\[
\mathbb{E} [|\ell(A(T_j), O) - \ell(A(T_{j,l}, O)) | \mid D_T, O'] \leq 2\beta_{n_T}.
\]
It follows from the definition of \(h\) that
\[
|h(A(T_j), O_i) - h(A(T_{j,l}, O_i))| \leq 4\beta_{n_T} + L \mathbb{1} \{ i = l \}.
\]
By using the identity \(\frac{1}{K} \sum_{j=1}^{K} \mathbb{1} \{ l \in T_j \} = \frac{n}{n_T}\) we get
\[
\Delta_l(D, O') \leq \frac{4\beta_{n_T} n_T}{n} + \frac{L}{n}.
\]
Thus by McDiarmid’s (Proposition A.1), we obtain, for $Z = f(D) - \mathbb{E}[f(D)]$, that

$$\mathbb{P}(Z \geq t) \leq \exp\left(\frac{-2nt^2}{(4\beta n_T + L)^2}\right).$$

Symmetrically, the event $-Z \geq t$ is subject to the same probability bound. It follows that

$$\mathbb{P}(|Z| \geq t) \leq 2 \exp\left(\frac{-2nt^2}{(4\beta n_T + L)^2}\right). \quad (B.4)$$

To derive an upper bound for $\mathbb{E}\left[D_A[D_{T_1:K}]\right]$, we use the fact that all the training sets have the same length so that

$$\mathbb{E}(D_A[D_{T_1:K}]) = \mathbb{E}\left[R[A(T_1)] - \hat{R}[A(T_1), T_1]\right].$$

Then, we use Lemma 7 from (Bousquet and Elisseeff 2002) ensuring that

$$\forall T \subset [n], \quad \mathbb{E}\left[R[A(T)] - \hat{R}[A(T), T]\right] = \mathbb{E}\left[\ell(A(T), O') - \ell(A(T^i), O')\right].$$

Where $A(T^i)$ is the learning rule $A$ trained on the sample $D_T \setminus \{O_i\} \cup \{O'\}$. Replacing the left side term by $\mathbb{E}\left[D_A[D_{T_1:K}]\right]$ and using Fact 2.1 gives

$$|\mathbb{E}[f(D)]| = |\mathbb{E}\left[D_A[D_{T_1:K}]\right]| \leq 2\beta n_T.$$ 

Since $|f(D)| \leq |Z| + 2\beta n_T$, we simply use (B.4) to reach the conclusion. \qed

**Remark B.1.** Applying Lemma B.2 with $T = [n]$ and $K = 1$ gives the following probability upper bound

$$\mathbb{P}\left(\left|\hat{R}[A([n]), [n]] - R[A([n])]\right| \geq t + 2\beta n_T\right) \leq 2 \exp\left(\frac{-2nt^2}{(L + 4\beta n)^2}\right).$$

Thus we retrieve the bound of Theorem 12 in (Bousquet and Elisseeff 2002). It turns out that Lemma B.2 can be seen as an extension of the latter Theorem to a wide class of CV estimates.

### C Detailed proofs

#### C.1 Proof of Fact 2.1

The result follows using the following decomposition,

$$|\ell(A(T), O) - \ell(A(T^i), O)| \leq |\ell(A(T), O) - \ell(A(T^i), O)| + |\ell(A(T^i), O) - \ell(A(T^i), O)| \leq 2\beta n_T.$$
C.2 Proof of Theorem 3.1

We proceed as described in the sketch of proof. Using equation 3.2, write
\[ \left| \hat{R}_{CV} [A, V_{1:n}] - R[A([n])] \right| \leq |D_{CV}| + |\text{Bias}|. \]

It remains to combine Lemma B.1, Fact 2.2, with the assumption that \( \beta_t \leq \frac{\lambda}{t} \) to obtain the desired result.

C.3 Proof of Theorem 4.1

We follow the steps described in the sketch of proof. To prove the boundedness of \( \ell \), notice that with \( P \)-probability one regarding \( O = (X, Y) \) we have that both \( Y \) and \( A(T)(X) \) belong to the interval \([0, MS_n]\), so that
\[ \ell(A[T], O) = |A(T)(X) - Y| \leq MS_n. \]

Now since \( 1/j \leq \int_{j-1}^{j} x^{-1}dx \),
\[ S_n = 1 + \sum_{j=2}^{n} (1/j) \leq 1 + \int_{1}^{n} x^{-1}dx = \log(n) + 1. \]

Since by assumption \( \log(n) \leq M \) we obtain \( \ell(A[T], O) \leq M(\log(n) + 1) \leq (M + 1)^2. \)

We now verify that the learning rule defined in (4.2) is \( (3\lambda/t) \) uniformly stable for \( t \leq n \).

First, notice that under the assumptions \( n \geq 2, 0 \leq \lambda \leq \frac{M}{2} \) and \( 0 \leq \epsilon \leq \frac{\lambda}{n} \), one has
\[ A(T)(x_m) \leq y_m, \]
where \( y_m = x_m + \sigma_m \epsilon \) (cf. eq 4.1). Thus, with probability one,
\[ \ell(A(T), O) = Y - A(T)(X). \quad \text{(C.1)} \]

Using Equation C.1 and the triangular inequality yields
\[ |\ell(A(T), O) - \ell(A(T^{\setminus j}), O)| \leq \lambda |S_{\min(m, n_T)} - S_{\min(m, n_T - 1)}| + 2\epsilon \]
\[ = \begin{cases} 2\epsilon + \frac{\lambda}{n_T} & \text{if } i = n_T \\ 2\epsilon & \text{otherwise} \end{cases} \]
\[ (\epsilon \leq \frac{\lambda}{n_T}) \leq \frac{3\lambda}{n_T}. \]

Consequently, \( A \) is \( \frac{3\lambda}{n_T} \) uniformly stable. Now, let us compute the generalization risk of our
algorithm. Since $P$ is the uniform distribution over $\mathcal{Z}$, we can write for any $T \subset [n]$

$$\mathcal{R}[\mathcal{A}(T)] = \mathbb{E}[\mathcal{A}(T), O | \mathcal{D}_T]$$

$$= \frac{1}{n} \sum_{x_m \in \mathcal{X}} \ell(\mathcal{A}(T), (x_m, y_m))$$

(By C.1) $$= \frac{1}{n} \sum_{m=1}^{n} (y_m - \mathcal{A}(T)(x_m))$$

$$= \frac{1}{n} \sum_{m=1}^{n} \left( MS_m - \lambda S_{\min(n_T,m)} + \varepsilon \text{sign}(\text{med}(\mathcal{D}_T) - x_m) \right).$$

Thus, one obtains by simple algebra

$$\mathcal{R}[\mathcal{A}(T)] - \mathcal{R}[\mathcal{A}([n])] \geq \frac{\lambda}{n} \sum_{m=(n_T+1)}^{n} (S_m - S_{n_T}) - 2\varepsilon. \tag{C.2}$$

To conclude the proof, it remains to derive a lower bound for the right-hand side term in the above display. To do so write

$$\frac{\lambda}{n} \sum_{m=(n_T+1)}^{n} (S_m - S_{n_T}) - 2\varepsilon = \frac{\lambda}{n} \sum_{m=(n_T+1)}^{n} \left( \sum_{j=(n_T+1)}^{m} \frac{1}{j} \right) - 2\varepsilon$$

$$\geq \frac{\lambda}{n^2} \sum_{m=(n_T+1)}^{n} (m - n_T - 1) - 2\varepsilon$$

$$\geq \frac{\lambda}{n^2} \sum_{m=1}^{n_T} m - 2\varepsilon$$

$$\geq \frac{\lambda}{2K^2} \frac{n_V}{n^2} - \frac{2\lambda}{n}$$

$$\geq \frac{\lambda}{2K^2} - \frac{2\lambda}{n}. \tag{C.3}$$

The first inequality comes from the fact that $\frac{1}{j} \geq \frac{1}{n}$; The second inequality comes from the fact that $n_V = n - n_T$; The third inequality comes from the fact that $\varepsilon \leq \frac{\lambda}{n}$; The last inequality comes from the fact that $(n_V = \frac{K}{n})$ for the K-fold scheme. Combining Inequalities C.2,C.3 gives

$$\frac{\lambda}{2K^2} - \frac{2\lambda}{n} \leq \mathcal{R}[\mathcal{A}(T)] - \mathcal{R}[\mathcal{A}([n])]. \tag{C.4}$$

On the other hand, by recalling that $\mathcal{R}[\mathcal{A}(T_j)] \geq \mathcal{R}[\mathcal{A}([n])]$ and applying the tower rule
yields
\[ \mathbb{E} \left[ \tilde{R}_{CV} [A, V_{1:K}] - R [A([n])] \right] = \mathbb{E} \left[ \frac{1}{K} \left( \sum_{j=1}^{K} R(A(T_j)) - R [A([n])] \right) \right] \]
\[ = \mathbb{E} \left[ \frac{1}{K} \left( \sum_{j=1}^{K} R(A(T_j)) - R [A([n])] \right) \right], \]
which, using C.4, gives the desired result.

C.4 Proof of Theorem 5.1

We proceed as described in the sketch of proof. First remind the error decomposition 5.2
\[ \tilde{R}_{CV} [A, V_{1:K}] - R [A([n])] = D_{A[1:T]} + n_T \left( D_{CV} - D_{A[T_1,K]} \right), \]
where \( D_{CV}, D_{A[T_1,K]} \) and \( D_{A[n]} \) are defined in 3.3, 5.4 and 5.3 respectively. Since \( n_T \leq n \), using the triangular inequality yields
\[ |\tilde{R}_{CV} [A, V_{1:K}] - R [A([n])]| \leq |D_{A[1:T]}| + |D_{CV}| + |D_{A[T_1,K]}|. \]
Combining lemma B.1 and B.2 regarding \( D_{CV} \) and \( D_{A[T_1,K]} \) with Remark B.1 regarding \( D_{A[n]} \), one obtains
\[ \mathbb{P} \left( |\tilde{R}_{CV} [A, V_{1:K}] - R [A([n])]| \geq t + 2(\beta_{n_T} + \beta_n) \right) \]
\[ \leq \mathbb{P} (|D_{CV}| \geq t/3) + \mathbb{P} (|D_{A[1:T]}| \geq t/3 + 2\beta_n) + \mathbb{P} (|D_{A[T_1,K]}| \geq t/3 + 2\beta_{n_T}) \]
\[ \leq 6 \exp \left( \frac{-2nt^2}{9(4\beta_{n_T} n_T + L)^2} \right). \quad (C.5) \]
By inverting, and using the assumption \( \beta_t \leq \frac{1}{t} \) one gets, with probability \( 1 - 6\delta \),
\[ |\tilde{R}_{CV} [A, V_{1:K}] - R [A([n])]| \leq 2\lambda \left( \frac{1}{n} + \frac{1}{n_T} \right) + 3(4\lambda + L) \sqrt{\frac{\log(1/\delta)}{2n}}, \]
which is the desired result.

C.5 Proof of Theorem 6.1

The proof of Theorem 6.1 relies on the following proposition,

Proposition C.1. Let \((A^{(m)})_{m \in M}\) be a family of algorithms where each learner \( A^{(m)} \) is \((\beta_{m,t})_{1 \leq t \leq n}\) uniform stable with respect to loss function \( 0 \leq \ell(g,O) \leq L \). Additionally, assume that, \(|M| < \infty\) and
\[ \forall m \in M ; \beta_{m,t} \leq \frac{M}{t}, \]
for some $M > 0$. Then one has, with probability at least $1 - 6\delta$,

$$
\sup_{m \in \mathcal{M}} \left| \hat{R}_{K\text{-fold}}^{\text{corr}} \left[ \mathcal{A}^{(m)}, V_{1:K} \right] - R \left[ \mathcal{A}^{(m)}([n]) \right] \right| \leq \frac{6M}{n} + 4(M + L)\sqrt{\frac{\log(|\mathcal{M}|/\delta)}{n}}.
$$

**Proof.** Using equation C.5 for the K-fold scheme ($n_T = n(K-1)/K$ with $K \geq 2$), and the fact that $\beta_{m,n} + \beta_{m,n_T} \leq (M/n)((2K-1)/(K-1))$ as well as $(2K-1)/(K-1) \leq 3$. One gets

$$
\forall m \in \mathcal{M}, \quad \mathbb{P} \left( \left| \hat{R}_{K\text{-fold}}^{\text{corr}} \left[ \mathcal{A}^{(m)}, V_{1:K} \right] - R \left[ \mathcal{A}^{(m)}([n]) \right] \right| \geq t + (6M/n) \right) \leq 6 \exp \left( \frac{-2nt^2}{9(4M + L)^2} \right),
$$

which gives by union bound

$$
\mathbb{P} \left( \sup_{m \in \mathcal{M}} \left| \hat{R}_{K\text{-fold}}^{\text{corr}} \left[ \mathcal{A}^{(m)}, V_{1:K} \right] - R \left[ \mathcal{A}^{(m)}([n]) \right] \right| \geq t + (6M/n) \right) \leq 6|\mathcal{M}| \exp \left( \frac{-2nt^2}{9(4M + L)^2} \right).
$$

Thus, by inverting, we obtain the desired result.

**Proof of Theorem 6.1** First, using the definition of $\hat{m}$ (eq 6.2) write

$$
\hat{R}_{K\text{-fold}}^{\text{corr}} \left[ \mathcal{A}^{(\hat{m})}, V_{1:K} \right] - \hat{R}_{K\text{-fold}}^{\text{corr}} \left[ \mathcal{A}^{(m^*)}, V_{1:K} \right] \leq 0.
$$

It follows that,

$$
R \left[ \mathcal{A}^{(\hat{m})}([n]) \right] - R \left[ \mathcal{A}^{(m^*)}([n]) \right] \leq R \left[ \mathcal{A}^{(\hat{m})}([n]) \right] - \hat{R}_{K\text{-fold}}^{\text{corr}} \left[ \mathcal{A}^{(\hat{m})}, V_{1:K} \right] + \hat{R}_{K\text{-fold}}^{\text{corr}} \left[ \mathcal{A}^{(m^*)}, V_{1:K} \right] - R \left[ \mathcal{A}^{(m^*)}([n]) \right]
$$

$$
\leq 2 \sup_{m \in \mathcal{M}} \left| \hat{R}_{K\text{-fold}}^{\text{corr}} \left[ \mathcal{A}^{(m)}, V_{1:K} \right] - R \left[ \mathcal{A}^{(m)}([n]) \right] \right|.
$$

It remains to use proposition C.1 and the proof is complete.

**D Uniform stability for randomized algorithms**

In this section we generalize the results from the main paper to the case of randomized algorithms. Let us start with reminding the concept of uniform stability for randomized learning algorithms introduced in (Elisseeff et al. 2005).

**Definition D.1.** An algorithm $A$ is said to be $(\beta_t)_{1 \leq i \leq n}$-uniform stable with respect to a loss function $\ell$ if, for any $T \subset [n]$, $i \in T$ and $O \in \mathcal{Z}$, the following holds

$$
\mathbb{E} \left[ \ell \left( A(T), O \right) - \ell \left( A(T \setminus i), O \right) \mid D_T, O \right] \leq \beta_{n_T}.
$$

**Remark D.1.** Note that the randomness in the latter expectation stems from the randomness in the algorithm $A$ only while the dataset $D_T$ and the observation $O$ are fixed.
Note that a similar version of Facts 2.1 and 2.2 still holds, more precisely, one has

**Fact D.1.** If an algorithm $A$ is $(\beta_t)_{1 \leq t \leq n}$ uniformly stable with respect to a loss function $\ell$ then, $A$ is $(2\beta_t)_{1 \leq t \leq n}$ change-one stable. In other words, for any $T \subset [n]$, $i \in T$ and $O, O' \in \mathcal{Z}$, the following holds

$$|E[\ell(A(T), O) - \ell(A(T'), O) | DT, O', O]| \leq 2\beta_{nT}.$$  

**Fact D.2.** Let $A$ be a decision rule which is $(\beta_t)_{1 \leq t \leq n}$ uniformly stable, additionally suppose that the sequence $(\beta_t)_{1 \leq t \leq n}$ is decreasing, then for any $T \subset [n]$ and $O \in \mathcal{Z}$, one has

$$|E[\ell(A([n]), O) - \ell(A(T), O) | D]| \leq (n - n_T)\beta_{nT}.$$  

We now derive upper bounds -in expectation- on the error induced by $\hat{R}_{CV}$ and $\hat{R}_{CV}^{corr}$.

**Theorem D.1.** Suppose that Assumption 1 holds with $\beta_n \leq \lambda n$, for some $\lambda > 0$. Then we have

$$E[\hat{R}_{CV}[A, V_{1:K}] - R[A([n])]] \leq \frac{\lambda n V}{n_T}.$$  

**Proof.** First, by applying the tower rule one has

$$E[\hat{R}_{CV}[A, V_{1:K}] - R[A([n])]] = E \left[ \frac{1}{K} \sum_{j=1}^{K} \hat{R}[A(T_j), V_j] - R[A([n])] \right]$$

$$= \frac{1}{K} \sum_{j=1}^{K} E \left[ \hat{R}[A(T_j), V_j] | DT_j] - R[A([n])] \right]$$

$$= \frac{1}{K} \sum_{j=1}^{K} E \left[ \ell(A(T_j, O) | DT_j] - R[A([n])] \right]$$

$$= \frac{1}{K} \sum_{j=1}^{K} E [E[\ell(A(T_j, O) - \ell(A([n], O)) | D]]. \quad (D.2)$$

The third line follows from the fact that $\ell(A(T), O_j)$ and $\ell(A(T), O)$ has the same law for all $j \in V$. This indeed verified since all the training sets $T_j$’s has the same length and the $O_j$’s are independent from $DT$. To obtain the desired result, it remains to combine Equation D.2 with fact D.1. \hfill \qed

Theorem D.1 yields the following control over the bias of the l.p.o.

**Corollary D.1 (l-p-o consistency).** Suppose that Assumption 1 holds with $\beta_n \leq \frac{\lambda}{n}$, for some $\lambda > 0$. Then, we have,

$$\left| E[\hat{R}_{lpo}[A, V_{1:K}] - R[A([n])]] \right| \leq \frac{\lambda p}{n - p}.$$  

Now let us prove that the bias corrected K-fold (cf. Eq (5.1)) is indeed consistent for randomized algorithms.
Theorem D.2 (Corrected K-fold consistency). Suppose that Assumption 1 holds with $\beta_n \leq \frac{\lambda}{n}$, for some $\lambda > 0$. Then, we have

$$\left| \mathbb{E} \left[ \hat{R}_{K\text{fold}}^{\text{corr}} [A, V_{1:K}] - R[A([n])] \right] \right| \leq \frac{2\lambda(2K - 1)}{Kn}.$$  

Proof. Combining the error decomposition 5.2 with the fact that $n_T = \frac{K - 1}{K} n$ we obtain

$$\hat{R}_{K\text{fold}}^{\text{corr}} [A, V_{1:K}] - R[A([n])] = D_A[n] + \frac{K - 1}{K} (D_{CV} - D_{A[T_1:K]}). \quad (D.3)$$

Using Theorem 2.2 in (Hardt et al. 2016), one obtains the twin inequality

$$|\mathbb{E} [D_A[n]]| \leq 2\beta_n$$
$$|\mathbb{E} [D_{A[T_1:K]}]| \leq 2\beta_{n_T}.$$  

Since $\mathbb{E}[D_{CV}] = 0$, Equation D.3 combined with the triangular inequality gives

$$\left| \mathbb{E} \left[ \hat{R}_{K\text{fold}}^{\text{corr}} [A, V_{1:K}] - R[A([n])] \right] \right| \leq 2 \left( \beta_n + \frac{(K - 1)\beta_{n_T}}{K} \right) \leq 2 (\beta_n + \beta_{n_T}). \quad (D.4)$$

It remains to use the assumption $\beta_t \leq \frac{\lambda}{t}$ and the proof is complete. \qed

We conclude this section by deriving an upper bound for the model selection problem,

Theorem D.3. Let $(A^{(m)})_{m \in \mathcal{M}}$ be a family of algorithms where each learner $A^{(m)}$ is $(\beta_{m,t})_{1 \leq i \leq n}$ uniform stable with respect to loss function $0 \leq \ell(g, O) \leq L$. Additionally, assume that $\beta_{m,t} \leq \frac{M}{t}$

for some $M > 0$. Then one has

$$\mathbb{E} \left[ R[A^{(m)}([n])] - R[A^{(m^*)}([n])] \right] \leq \frac{4M(2K - 1)}{Kn},$$

where $m^*$ and $\hat{m}$ are defined by Equations 6.1, 6.2 respectively.

Proof. First, using Equation D.4, one obtains, for all $m \in \mathcal{M}$,

$$\left| \mathbb{E} \left[ \hat{R}_{K\text{fold}}^{\text{corr}} [A^{(m)}, V_{1:K}] - R[A^{(m)}([n])] \right] \right| \leq 2 (\beta_{m,n} + \beta_{m,n_T}) \leq \frac{2M(2K - 1)}{Kn}.$$  

So that

$$\sup_{m \in \mathcal{M}} \left| \mathbb{E} \left[ \hat{R}_{K\text{fold}}^{\text{corr}} [A^{(m)}, V_{1:K}] - R[A^{(m)}([n])] \right] \right| \leq \frac{2M(2K - 1)}{Kn}. \quad (D.5)$$
On the other hand, Inequality C.6 yields
\[
\mathbb{E} \left[ \mathcal{R} [A^{(\hat{m})}(\langle n \rangle)] - \mathcal{R} [A^{(m^*)}(\langle n \rangle)] \right] \leq \mathbb{E} \left[ \mathcal{R} [A^{(\hat{m})}(\langle n \rangle)] - \hat{\mathcal{R}}_{\text{Kfold}}^{\text{corr}} [A^{(\hat{m})}, V_1:K] \right] \\
+ \mathbb{E} \left[ \hat{\mathcal{R}}_{\text{Kfold}}^{\text{corr}} [A^{(m^*)}, V_1:K] - \mathcal{R} [A^{(m^*)}(\langle n \rangle)] \right] \\
\leq 2 \sup_{m \in M} \left| \mathbb{E} \left[ \hat{\mathcal{R}}_{\text{Kfold}}^{\text{corr}} [A^{(m)}, V_1:K] - \mathcal{R} [A^{(m)}(\langle n \rangle)] \right] \right|.
\]
Thus, by Inequality D.5, one has
\[
\mathbb{E} \left[ \mathcal{R} [A^{(\hat{m})}(\langle n \rangle)] - \mathcal{R} [A^{(m^*)}(\langle n \rangle)] \right] \leq \frac{4M(2K - 1)}{Kn},
\]
which concludes the proof. \qed