Cross validation for rare events

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Abstract

We derive sanity-check bounds for the cross-validation (CV) estimate of the generalization risk for learning algorithms dedicated to extreme or rare events. We consider classification on extreme regions of the covariate space, a problem analyzed in Jalalzai \textit{et al.} 2018. The risk is then a probability of error conditional to the norm of the covariate vector exceeding a high quantile.

Establishing sanity-check bounds consist in recovering bounds regarding the CV estimate that are of the same nature as the ones regarding the empirical risk. We achieve this goal both for K-fold CV with an exponential bound and for leave-p-out CV with a polynomial bound, thus extending the state-of-the-art results to the modified version of the risk which is adapted to extreme value analysis.

1 Introduction

Cross-validation (CV) is a most popular tool for estimating the generalization risk of machine learning (ML) algorithms. It is also the mainstream approach for hyper-parameters selection. Despite its widespread usage, the theoretical properties of CV estimates are notoriously difficult to establish due to the lack of independence between the different terms of the average involved in a CV scheme, see \textit{e.g.} Arlot and Celisse 2010 for a survey of CV for model selection or Wager 2020; Bates \textit{et al.} 2021 and the reference therein for recent discussions. In this paper we consider CV for risk estimation concerning specific ML algorithms dedicated to the analysis of rare events. More precisely the learning problems we have in mind involve \textit{i.i.d.} data \( Z_i, i \leq n \) in a sample space \( Z \subset \mathbb{R}^d \), and a low probability region \( \Lambda \subset Z \), typically \( \Lambda = \{ z \in Z : \| z \| > t_\alpha \} \) for some (semi)-norm \( \| \cdot \| \) and a large threshold \( t_\alpha \) chosen as the \( (1 - \alpha) \)-quantile of \( \| Z \| \). In such a context, it is natural to measure the performance of an algorithm in terms of an expected loss, \textit{conditional} to the rare event \( \| Z \| > t_\alpha \). Doing so allows to focus on extreme events with potentially tremendous societal impact. The price to pay is that the predictions issued from such an algorithm are theoretically guaranteed in the tail regions only. It should thus be coupled with a standard algorithm dedicated to the treatment of moderate events \( \{ \| Z \| < t_\alpha \} \), with a classical risk function.
Extreme Values. Analyzing rare events in the distributional tail is the main concern of Extreme Value Theory (EVT) (De Haan and Ferreira 2006). Under appropriate assumptions i.e. regular variation of the distribution of $Z$ (Bingham et al. 1989; Resnick 2013; Hult and Lindskog 2006), for some well-chosen normalization $b(t)$ the rescaled variable $b(t)Z$, conditional to $\|Z\| > t$, converges to a limiting distribution as $t \to \infty$, in a wide variety of settings ranging from univariate random variables to general complete metric spaces (Hult and Lindskog 2006), structured data such as Markov trees (Segers 2020), time series (Basrak and Segers 2009; Planinić and Soulier 2018) or continuous processes (Ferreira and De Haan 2014). An abundant literature is devoted to statistical implementation of EVT, motivated by a wide variety of applications related to risk management (Beirlant et al. 2006; Embrechts et al. 2013). Various summaries of the tail behavior are estimated using a sub-sample of size $k = k(n)$ made of the largest observations at hand. In this context the probability of the rare (=extreme) class is of order $\alpha = k/n$. The vast majority of existing theoretical results are obtained in an asymptotic framework: $n, k \to \infty$, $k/n \to 0$. In this context a tail empirical process comes into play and the rates of convergence of EVT functional estimators (such as tail index estimators) are typically of order $O(1/\sqrt{k})$ (see e.g. De Haan and Ferreira 2006, chap. 3,4).

Extremes and statistical learning. It is only recently that statistical learning viewpoints upon EVT have been developed with non-asymptotic guarantees regarding the statistical error of specific estimators or algorithms. Concentration inequalities for order statistics established in Boucheron and Thomas 2012 are leveraged in Boucheron and Thomas 2015 to choose $k$ in an adaptive manner for tail index estimation, in the univariate, i.i.d. case. Goix et al. 2015 obtain a uniform bound over a Vapnik-Chervonenkis (VC) class of sets regarding the deviations of the conditional empirical measure $P_{n,\alpha} = \frac{1}{n\alpha} \sum_{i=1}^{n} 1\{Z_i \in (\cdot \cap A)\}$, scaling as $O(1/\sqrt{n\alpha}) = O(1/\sqrt{k})$ w.r.t. the sample size. Their result improves by a factor $\sqrt{\alpha}$ over the naive bound obtained when dividing by $\alpha$ the standard VC inequality, see Bousquet et al. 2003, Th. 2. It also improves over more sophisticated re-normalized VC inequalities (Bousquet et al. 2003, Th. 7) by replacing a $\log(n)$ term with a (more natural) $\log(n\alpha) = \log(k)$ term.

Several ML algorithms incorporating (multivariate) EVT have been proposed over the past few years motivated by essential issues such as dimensionality reduction and/or anomaly detection (Goix et al. 2016, 2017; Thomas et al. 2017; Chiapino and Sabourin 2016; Drees and Sabourin 2021; Jalalzai and Leluc 2021, see also the review papers Engelke and Ivanovs 2021; Suboh and Aziz 2020), data augmentation (Jalalzai et al. 2020), adversarial simulation (Bhatia et al. 2021), and classification in extreme regions (Jalalzai et al. 2018, 2020). Most of these approaches come with tuning parameters, in addition to $k$ which choice is known to be difficult. Furthermore estimating the (conditional) generalization risk is all the more desirable in an EVT context because fewer training data are available, by construction. CV is a natural idea for such purposes.

Contributions. To our best knowledge, the present work is the first of its kind envisioning CV for algorithms related to EVT from a theoretical perspective.

We limit ourselves to the latter cited framework (classification in extreme regions, Jalalzai et al. 2018). Indeed classification by means of empirical risk minimization (ERM) is one of
the most illustrative example of ML task. We consider the problem of estimating the generalization risk of an ERM classifier, conditional to a rare event (see Definition 2.1) which plays a central role in ML algorithms dedicated to extremes. Our contributions may be summarized as follows: we obtain sanity check bounds (Kearns and Ron 1999; Cornec 2009, 2017) regarding the deviations of the CV estimate, that is, bounds that are of the same order of magnitude as the ones regarding the empirical risk itself. More precisely, we provide two new results:

(i) an exponential probability bound involving the size of the validation set, which yields a sanity check bound for the K-fold CV scheme but not the leave-p-out (l.p.o.) scheme as the size of the validation set in this case remains constant, equal to p;

(ii) a polynomial upper bound, which outperforms the exponential one in the case of the l.p.o. because the associated remainder term only involves the size of the training set.

Our techniques of proof borrow ideas from Cornec 2009, 2017 for the error decomposition of the K-fold CV scheme, from Kearns and Ron 1999 for the l.p.o. error, from Goix et al. 2015 for incorporating the probability of the considered class within the upper bounds. In particular we use a Bernstein-type inequality proved in McDiarmid 1998 which is also exploited in Goix et al. 2015; Clémencron et al. 2021; Drees and Sabourin 2021.

Limitations and further work. Sanity check bounds are difficult to improve upon without further assumptions regarding algorithm stability, e.g. loss stability as introduced in Kumar et al. 2013, where the variance of the K-fold CV is shown to be K-times smaller than that of the empirical risk. A lead for further research would be to consider such wider classes of algorithms, for which various stability hypotheses replace advantageously the assumption of finite VC dimension (see e.g. Kearns and Ron 1999; Bousquet and Elisseeff 2001, 2002).

Another promising avenue would be to consider unsupervised problems which are the main field of application for EVT. Also, while we limit ourselves to risk estimation, we hope that our work can pave the way towards a theoretical understanding of CV-based hyper-parameter selection in EVT algorithms.

Finally, even though our work is motivated by the EVT framework, no regular variation assumption is needed for our results to hold regarding CV risk estimates, and the precise definition of the rare class A is unimportant, only the small probability α is. Thus we believe that our results and techniques of proof could serve in other ML contexts involving a rare class, such as imbalanced multi-class classification where the learner must distinguish between several minority classes.

Outline. The statistical framework envisioned in this project is introduced in Section 2. Our main results Theorem 3.1 and 4.1 are presented respectively in Section 3 and Section 4. Intermediate results are gathered in Section 5. Additional technical results are deferred to the supplementary material (Section A) as well as some detailed proofs (Section B).
2 Extreme values, extreme risk and cross-validation: framework

Let \( O = (X, Y) \) be a random vector valued in \( Z = \mathcal{X} \times \mathcal{Y} \), having distribution \( P \). Let \( 0 < \alpha \ll 1 \), and let \( t_\alpha \) be the \( 1 - \alpha \) quantile of \( \|X\| \). Using \( t_\alpha \), one can define a ‘rare region’ (rare since \( \alpha \ll 1 \)) by \( \|X\| \geq t_\alpha \). For simplicity we assume that \( \alpha n = k \) is an integer, where \( n \) is the training sample size. Given a class of discrimination rules \( G \), define a loss function \( c : G \times Z \rightarrow \mathbb{R} \). Following Jalalzai et al. 2018 the risk of \( g \in G \) over the previous rare region is defined as

\[
R_\alpha(g) = \mathbb{E}[c(g, O) \mid \|X\| \geq t_\alpha].
\]

Let \( D_n = (O_1, \ldots, O_n) \) be a collection of independent and identically distributed random vectors with common distribution \( P \). Given a subsample \( S \subset \{1, \ldots, n\} \), the risk estimate based on \( S \) is given by

\[
\hat{R}_\alpha(g, S) = \frac{1}{\alpha n_S} \sum_{i \in S} c(g, O_i) \mathbb{1}\{\|X_i\| > \|X_{\lfloor \alpha n \rfloor}\}.
\]

where \( n_S = \text{card}(S) \) and \( \|X_1\| \geq \ldots \geq \|X_n\| \) are the (reverse) order statistics of the sample \((\|X_i\|)_{i=1,\ldots,n}\). Our main results hold under assumptions 1 to 2 introduced below.

**Assumption 1** (ERM algorithm). The learning rule \( \Psi_\alpha \) is defined as the empirical risk minimizer,

\[
\Psi_\alpha(S) = \arg \min_{g \in G} \hat{R}_\alpha(g, S).
\]

Based on the previous definition, the Hold-out estimator of the risk of the learning rule \( \Psi_\alpha \) with validation set \( V \subset \{1, \ldots, n\} \) and training set \( T = \{1, \ldots, n\} \setminus V \) takes the simple form \( \hat{R}_\alpha(\Psi_\alpha(T), V) \). Given a family of validation sets in \( \{1, \ldots, n\}, V_1:K = (V_j)_{j=1,\ldots,K} \), the CV estimator of the risk of \( \Psi_\alpha \) is

\[
\hat{R}_{CV,\alpha}(\Psi_\alpha, V_1:K) = \frac{1}{K} \sum_{j=1}^K \hat{R}_\alpha(\Psi_\alpha(T_j), V_j),
\]

where \( T_j = \{1, \ldots, n\} \setminus V_j \). In the sequel we shall often refer to \( V_1:K \) as the sequence of masks because the validation sets are masked at the training step. 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 \( n_V = n/K \). We also need the sequence of masks to satisfy a certain balance condition which is expressed below.

**Assumption 2** (Mask property). The sequence of masks \( V_1, V_2, \ldots V_K \) satisfies

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

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

\[
\frac{1}{K} \sum_{j=1}^K \mathbb{1}\{l \in V_j\} = \frac{n_V}{n} \quad \forall l \in [1, n].
\]
The next lemma ensures that Assumption 2 holds true for the standard CV procedures (K-fold and l.p.o) and that condition similar to (2.5) is also valid for the training sets $T_j$.

**Lemma 2.1.** If $K$ divides $n$, for the leave-one-out, leave-p-out, and K-fold procedures, the sequence of masks $V_{1:K}$ satisfies Assumption 2. Also the the training sets $T_{1:K}$ satisfy

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

**Proof:** See Appendix B.1 \qed

**Remark 2.1.** The condition that $K$ divides $n$ is required for the K-fold CV only, in order to ensure that $\text{card}(V_j) = n_V$ for all $j$. However straightforward extensions of our results can be obtained in the case where $K$ does not divide $n$ at the price of some notational complexity.

We now introduce two assumptions relative to the function class $G$ and the cost function $c$. They shall be useful to control the fluctuation of the underlying empirical process. First we require the following standard complexity restriction on the family of functions $(x, y) \mapsto c(g(x), y)$ when $g$ lies in $G$.

**Assumption 3** (finite VC dimension). The family $G$ of classifiers and the cost function $c$ are such that the class of functions $o \mapsto c(g, o) = c(g(x), y)$ on $Z$ has a finite VC-dimension $\nu_G$, i.e. the family of subgraphs $\{(x, y, t) : t < c(g(x), y)\} : t \in \mathbb{R}, (x, y) \in Z, g \in G$ has Vapnik dimension $\nu_G$.

Since part of our proofs rely on Giné and Guillou 2001, we may rather assume directly that the covering number for the $L^2$ norm of this family of functions decrease polynomially (with exponent $\nu_G$) (see their condition (2.1)). This would not change the results. This condition is sometimes easier to check in practice.

For simplicity and in view of our focus on binary classification, we limit ourselves to a cost function bounded by 1. Our result may be extended to any bounded cost function at the price of a multiplicative scaling factor.

**Assumption 4** (Normalized cost function). The cost function $c$ is non-negative and bounded by 1,

$$
0 \leq c(g, O) \leq 1 \quad \forall (g, O) \in G \times Z.
$$

This hypothesis is clearly satisfied for the Hamming loss $c(g, O) = \mathbb{1}\{g(X) \neq Y\}$.

### 3 Exponential bounds for K-fold CV estimates in rare regions

Our first main result Theorem 3.1 below holds true for any CV procedure under assumptions 1 - 4. The leading term of the provided upper bound is $O(\sqrt{\frac{V_G}{n_V\alpha}})$. In the case of the K-fold

$$
\frac{1}{n_V} = O\left(\frac{1}{n}\right).
$$

Thus, the bound of Theorem 3.1 becomes $O(\sqrt{\frac{V_G\log(1/\delta)}{n\alpha}})$. The latter bound is indeed a sanity check bound as it matches (up to unknown multiplicative constants) the
one relative to the empirical risk conditional to a rare event established in Jalalzai et al. 2018, Th. 2, where \( k = n\alpha \). Similar rates are obtained in an unsupervised framework e.g. in Goix et al. 2015; Drees and Sabourin 2021; Clémençon et al. 2021. All these results match the asymptotic rate of convergence for tail empirical processes, see e.g. Einmahl and Mason 1988.

We shall use the notation \( S_n = \{1, \ldots n\} \) to refer to the full index set. Hence, \( \Psi_\alpha(S_n) \) denotes the algorithms trained on \( D_n \).

**Theorem 3.1** (Exponential CV bound for rare events). Under assumption 1, 2, 3, 4, we have, with probability \( 1 - 15\delta \),

\[
\left| \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_\alpha(\Psi_\alpha(S_n)) \right| \leq E_{CV}(n_T, n_V, \alpha) + \frac{20}{3n\alpha} \log(\frac{1}{\delta}) + 20\sqrt{\frac{2}{n\alpha} \log(\frac{1}{\delta})},
\]

where we put

\[
E_{CV}(n_T, n_V, \alpha) = M \sqrt{V_1} \left( \frac{1}{\sqrt{nV\alpha}} + \frac{4}{\sqrt{nT\alpha}} \right) + \frac{5}{nT\alpha},
\]

for some universal constant \( M > 0 \).

**Sketch of the proof.** Introduce the pseudo-empirical risk

\[
\hat{R}_\alpha(g, S) = \frac{1}{\alpha nS} \sum_{i \in S} c(g, O_i) \mathbb{1}\{\|X_i\| > t_\alpha\}.
\]

(3.1)

Notice that when the distribution of \( \|X\| \) is unknown, \( \hat{R}_\alpha \) is not observable and only \( \hat{R}_\alpha \) is a genuine statistic. However \( \hat{R}_\alpha \), will serve as an intermediate quantity in the proofs.

Define the average ‘true’ risk of the family \((\Psi_\alpha(T_j))_{0 \leq j \leq K}\) by

\[
R_{CV,\alpha}(\Psi_\alpha, V_{1:K}) = \frac{1}{K} \sum_{j=1}^K R_\alpha(\Psi_\alpha(T_j))
\]

(3.2)

and the average pseudo-empirical risk by

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

(3.3)

Using the previous quantities, write the following decomposition

\[
\left| \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_\alpha(\Psi_\alpha(S_n)) \right| \leq D_{tn} + D_{cv} + Bias,
\]

(3.4)

with

\[
D_{tn} = |\hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K})|,
\]

(3.5)

\[
D_{cv} = |\hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_{CV,\alpha}(\Psi_\alpha, V_{1:K})|,
\]

(3.6)

\[
Bias = |R_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_\alpha(\Psi_\alpha(S_n))|.
\]

(3.7)
The remainder of the proof (see Section B.4) consists in deriving upper bounds for each terms of the error decomposition (3.4), from which the result follows. The term $D_{tv}$ measures the deviation between the cross validation estimator when using the order statistics and the cross validation estimator when using the ‘true’ level $t_{\alpha}$, which can be bounded using Bernstein inequality, taking advantage of the small variance of the random indicator function $\mathbb{1}\{\|X\| > t_{\alpha}\}$. The term $D_{cv}$ measures the deviations of $\hat{R}_{CV,\alpha}(\Psi_{\alpha}, V_{1:K})$ from its mean. It is controlled by a uniform bound (over the class $G$) on the deviations of the empirical risk evaluated on the validation sample. To do so we follow standard arguments leading to a bound on such deviations on low probability regions (as e.g. in Goix et al. 2015; Jalalzai et al. 2018). Finally the term Bias is the bias of the cross validation procedure, the control of which relies on the specific nature (ERM) of the considered learning algorithm. Indeed in this context the bias may be upper bounded in terms of the supremum deviations of the empirical risk evaluated on the training sets $T_j$.

Theorem 3.1 can be used to obtain exponential bounds for the $K$-fold CV estimate. From Lemma 2.1, Assumption 2 regarding the sequence of masks $V_{1:K}$ holds true for the $K$-fold CV procedure. Consequently Theorem 3.1 applies with $n_V = n/K$ and $n_T = n - n_V = K - 1$. In the following corollary, $V_{1:K}^{K\text{-fold}}$ denote the sequence of masks associated to the $K$-fold.

**Corollary 3.1.** Under the assumptions of Theorem 3.1, the $K$-fold (with $K \geq 2$) CV estimate for the conditional risk (2.1) satisfies with probability $1 - 15\delta$,

$$\left| \hat{R}_{CV,\alpha}(\Psi_{\alpha}, V_{1:K}^{K\text{-fold}}) - R_{\alpha}(\Psi_{\alpha}(S_n)) \right| \leq E_{K\text{-fold}}(n, K, \alpha) + \frac{20}{3n\alpha} \log\left(\frac{1}{\delta}\right) + 20\sqrt{\frac{2}{n\alpha}} \log\left(\frac{1}{\delta}\right),$$

with, for some universal constant $M > 0$,

$$E_{K\text{-fold}}(n, K, \alpha) = 5M \sqrt{\frac{V_{\alpha} K}{n\alpha}} + \frac{5K}{(K-1)n\alpha}.$$

Despite the satisfactory sanity check bound obtained thus far for the $K$-fold (Corollary 3.1), note that the term $O\left(\sqrt{\frac{V_{\alpha}}{n_{T}\alpha}}\right)$ in the upper bound of Theorem 3.1 does not even converge to 0 in the l.p.o. setting because the size $n_V$ of the validation set remains constant, equal to $p$. Thus, Theorem 3.1 is not adapted to the latter type of CV schemes. In the next section we obtain (Theorem 4.1) an alternative upper bound involving only the size $n_T$ of the training set which allows to cover the l.p.o. case.

## 4 Polynomial bounds for l.p.o. CV estimates in rare regions

As discussed at the end of Section 3, Theorem 3.1 provides trivial bounds for CV schemes with small test size. In contrast our second main result (Theorem 4.1 below) yields a sanity-check bound for a wider class of CV procedures, including leave-one-out and l.p.o.. In particular, we show that, with high probability, the error is at most $O\left(\sqrt{\frac{V_{\alpha}}{n_{T}\alpha}}\right)$. Most -if not all- CV procedures satisfy $\frac{1}{n_T} = O\left(\frac{1}{n}\right)$ and the latter bound is thus of order $O\left(\frac{V_{\alpha}}{n\alpha}\right)$. 

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Theorem 4.1 (Polynomial cross-validation bounds for rare events). Under assumptions 1, 2, 3, 4 one has with probability $1 - 18\delta$,

$$\left| \hat{R}_{CV,\alpha}(\Psi_\alpha , V_{1:K}) - R_\alpha (\Psi_\alpha (S_n)) \right| \leq E'_{CV}(n_T,\alpha) + \frac{1}{\delta n_T}(5M\sqrt{V_\delta} + M_5),$$

where $M, M_5 > 0$ are universal constants, $M$ is the same as in Theorem 3.1 and

$$E'_{CV}(n_T,\alpha) = \frac{5M\sqrt{V_\delta}}{\sqrt{n_T\alpha}} + \frac{9}{n_T\alpha}.$$

Sketch of the proof. First write

$$\left| \hat{R}_{CV,\alpha}(\Psi_\alpha , V_{1:K}) - R_\alpha (\Psi_\alpha (S_n)) \right| \leq \text{Bias} + \left| \hat{R}_{CV,\alpha}(\Psi_\alpha , V_{1:K}) - R_{CV,\alpha}(\Psi_\alpha , V_{1:K}) \right|,$$

where Bias is defined by (3.7).

The upper bound for the term Bias obtained in the proof of Theorem 3.1 is of order $O(1/\sqrt{n_T\alpha})$, see (B.14) in the supplement for details. Since $1/n_T = O(1/n)$ in the CV schemes that we consider, the latter bound is sufficient to obtain a sanity check bound. However, in that proof, the term $|\hat{R}_{CV,\alpha}(\Psi_\alpha , V_{1:K}) - R_{CV,\alpha}(\Psi_\alpha , V_{1:K})|$ is upper bounded by the sum $D_{bs} + D_{cv}$ defined in (3.5) and (3.6). The probability upper bound for the latter term involves a term of order $O(1/\sqrt{n_T\alpha})$, see (B.5) in the supplement, which is not satisfactory for small $n_V$. Therefore one needs an alternative control for $|\hat{R}_{CV,\alpha}(\Psi_\alpha , V_{1:K}) - R_{CV,\alpha}(\Psi_\alpha , V_{1:K})|

The main ingredient to proceed is the following Markov-type inequality

$$\mathbb{P}(\hat{R}_{CV,\alpha}(\Psi_\alpha , V_{1:K}) - R_{CV,\alpha}(\Psi_\alpha , V_{1:K}) \geq t) \leq \frac{\mathbb{E}(\left| \hat{R}_{\alpha}(\Psi_\alpha (S_n), S_n) - \hat{R}_{\alpha}(\Psi_\alpha (S_n)) \right|)}{t} + \frac{\mathbb{E}(D_{bs} + \text{Bias})}{t},$$

which holds true under the stipulated assumptions. The proof is deferred to the supplement (Lemma A.2). It is shown in Section B.5 from the supplement that $\mathbb{E}(\text{Bias})$ and $\mathbb{E}(D_{bs})$ are both upper bounded by $O(1/\sqrt{n_T\alpha})$ (inequalities B.17 B.18). In addition the probability upper bound on the supremum deviations on the rare region (Lemma A.3) also used in the proof of Theorem 3.1 shows that the latter quantity is sub-Gaussian, which yields (Vershynin 2018, Proposition 2.5.2) an upper bound for $\mathbb{E}(\left| \hat{R}_{\alpha}(\Psi_\alpha (S_n), S_n) - \hat{R}_{\alpha}(\Psi_\alpha (S_n)) \right|)$ of the same order of magnitude as the other terms in the r.h.s. of (4.2).

The final step of the proof is to derive a probability upper bound for the opposite of the l.h.s. of (4.2), that is $R_{CV,\alpha}(\Psi_\alpha , V_{1:K}) - \hat{R}_{CV,\alpha}(\Psi_\alpha , V_{1:K})$. We use the fact (proved in Lemma A.1) that the CV risk estimate $\hat{R}_{CV,\alpha}(\Psi_\alpha , V_{1:K})$ is always larger than the empirical risk $\hat{R}_{\alpha}$ evaluated on its minimizer $\Psi_\alpha (S_n)$, thus

$$R_{CV,\alpha}(\Psi_\alpha , V_{1:K}) - \hat{R}_{CV,\alpha}(\Psi_\alpha , V_{1:K}) \leq R_{CV,\alpha}(\Psi_\alpha , V_{1:K}) - \hat{R}_{\alpha}(\Psi_\alpha (S_n), S_n) \leq \text{Bias} + \left| R_\alpha (\Psi (S_n)) - \hat{R}_\alpha (\Psi_\alpha (S_n), S_n) \right|,$$

where the last inequality follows from the definition of Bias in (3.7) and the triangle inequality. From the proof of Theorem 3.1, Bias admits a probability upper bound involving only $n$ and
The second term in the r.h.s. of (4.3) is less than the supremum deviations of the empirical risk \( \hat{R}_\alpha \), which shares the same property (Lemma A.3). Summing up the upper bounds for each term of the r.h.s. of (4.2) and (4.3) concludes the proof, see Section B.5 in the supplement for details.

Using Theorem 4.1 and following the same steps as in the proof of corollary 3.1, we obtain a sanity-check guarantee regarding leave-p-out estimates. In the following statement, \( V_{1:K}^{lpo} \) denotes the sequence of masks associated with the l.p.o. CV scheme.

**Corollary 4.1** (leave-p-out sanity check for rare events). Under the assumptions of Theorem 4.1, the l.p.o. CV estimate for the conditional risk (2.1) satisfies with probability \( 1 - 15\delta \),

\[
| \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}^{lpo}) - R_\alpha(\Psi_\alpha(S_n)) | \leq E_{lpo}(n, p, \alpha) + \frac{1}{\delta \sqrt{(n-p)\alpha}}(5M \sqrt{V_G} + M_5),
\]

where

\[
E_{lpo}(n, p, \alpha) = 9M \sqrt{\frac{V_G}{(n-p)\alpha}} + \frac{9}{(n-p)\alpha}.
\]

**Remark 4.1.** [Tightness of the polynomial bound] A natural question to ask is whether or not the polynomial rate (w.r.t. the probability \( \delta \)) is tight concerning the l.p.o. CV scheme. The answer is yes, in the ERM context, in the general case (that is with a classical risk function with \( \alpha = 1 \)). Indeed Kearns and Ron 1999 show that, without further assumptions on the algorithm \( \Psi \) and the cost function \( c \), the bound \( 1/\delta \) can be attained. We conjecture that the same is true for \( \alpha < 1 \), leaving this question for further work.

**Remark 4.2** (Comparison between the bounds from theorems 3.1 and 4.1). Although Theorem 4.1 also applies to the K-fold, the bound provided by Theorem 3.1 is sharper for this particular CV scheme for small values of \( \delta \) due to its exponential nature. In other words Theorem 4.1 has a greater level of generality than Theorem 3.1 because the upper bound in the latter involved \( nV \), contrarily to the former. The price to pay is a slower tail decay (polynomial versus exponential).

## 5 Intermediate results

In this section we gather the main intermediate results involved in the proofs of our main results theorems 3.1 and 4.1, which are of interest in their own.

A key tool to our proofs is a Bernstein-type inequality relative to the deviation of a generic random variable \( Z = f(O_1, \ldots, O_n) \) from its mean (McDiarmid 1998) that we recall in the supplement for convenience (Proposition A.1). The control of the deviations involves both a maximum deviation term and a variance term. We leverage this result to control the deviations of the pseudo-empirical risk \( \hat{R}_\alpha \) defined in (3.1) averaged over the \( K \) validation sets \( V_{1:K} \). These deviations are embodied by the random variable \( Z \) defined in Lemma 5.1, Equation (5.1), which is a key quantity when analysing the deviations of any CV risk estimate as revealed by an inspection of the proofs in the supplement. Controlling the deviations of \( Z \) is the main purpose of this section.
Lemma 5.1. Let $D_n = (O_1, O_2, \ldots, O_n) \in \mathcal{X}^n$ be a sequence of random variables, and $V_1, V_2, \ldots, V_K$ a sequence of masks that verifies Assumption 2 with size $n_V$. Moreover, suppose that assumptions 3 and 4 regarding the class $\mathcal{G}$ and $c$ hold. Define

$$Z = \frac{1}{K} \sum_{j=1}^{K} \sup_{g \in \mathcal{G}} |\tilde{R}_\alpha(g, V_j) - R_\alpha(g)|,$$

where $\tilde{R}_\alpha$ is defined by Equation 3.1. Then the random variable $Z$ satisfies the Bernstein-type inequality

$$P(Z - E(Z) \geq t) \leq \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right).$$

Proof: The reader is referred to Appendix B.2.

To obtain a genuine probability bound on $Z$ via the latter lemma, one also needs to control the term $E(Z)$. This is the purpose of the next lemma, the spirit of which is similar to Lemma 14 in Goix et al. 2015. The main difference w.r.t. to the latter reference is that we handle any bounded cost function (not only the Hamming loss), using a bound for Rademacher averages from Giné and Guillou 2001 which applies in this broader setting.

Lemma 5.2. In the setting of Lemma 5.1, $Z$ satisfies

$$E(Z) \leq \frac{M \sqrt{V_G}}{\sqrt{\alpha n V}}.$$

where $M > 0$ is a universal constant.

Proof: See Appendix B.3

The following probability upper bound for $Z$ follows immediately by combining Lemma 5.1 and Lemma 5.2.

Corollary 5.1. In the setting of Lemma 5.1, we have

$$P \left( Z - \frac{M \sqrt{V_G}}{\sqrt{\alpha n V}} \geq t \right) \leq \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right),$$

where $Z$ is defined in (5.1).

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 Appendix A Additional results

This section gathers generic concentration tools and technical intermediate results that are necessary to the proofs of our main results.

A.1 Generic tools

First, we recall the following McDiarmid’s extension of Bernstein inequality (Theorem 3.8 in McDiarmid 1998).

**Proposition A.1.** For a sequence of observations \((O_1, O_2, \ldots, O_n) \in \mathbb{Z}^n\) and some fixed values \(o_{1:l} = (o_1, o_2, \ldots, o_l)\) and for some measurable function \(f : \mathbb{Z}^n \to \mathbb{R}\), let \(Z = f(O_1, O_2, \ldots, O_n)\) and define for \(l \in [1, n]\):

1. \(f_l(o_1, o_2, \ldots, o_l) = \mathbb{E}(Z \mid O_1 = o_1, O_2 = o_2, \ldots, O_l = o_l)\),

2. \(\Delta_l(o_1, o_2, \ldots, o_{l-1}, o_l) = f_l(o_1, o_2, \ldots, o_{l-1}, o_l) - f_{l-1}(o_1, o_2, \ldots, o_{l-1})\), (the positive deviations)

3. \(D := \max_{l=1, \ldots, n} \sup_{o_1, \ldots, o_{l-1} \in \mathcal{X}} \sup_{o \in \mathcal{X}} \Delta_l(o_1, \ldots, o_{l-1}, o)\), (the maximum positive deviation)

4. \(\sigma^2_l(o_{1:l-1}) = \operatorname{Var}[\Delta_l(O_1, O_2, \ldots, O_{l-1}, O') \mid O_1 = o_1, O_2 = o_2, \ldots, O_{l-1} = o_{l-1}]\), where \(O'\) is an independent copy of \(O_1\),

5. \(\sigma^2 = \sum_{l=1}^n \sup_{o_{1:l-1} \in \mathcal{X}^{l-1}} \sigma^2_l(o_{1:l-1})\) (the maximum sum of variances).

Then we have

\[
P(Z - \mathbb{E}[Z] > t) \leq \exp\left(-\frac{t^2}{2(\sigma^2 +Dt/3)}\right).
\]

We also recall Proposition 2.5.2 from Vershynin 2018, which provides an upper bound for the expectation of sub-Gaussian random variables.
Proposition A.2. Let $X$ be a real valued random variable and suppose that $\mathbb{P}(X \geq t) \leq C_1 \exp\left(-t^2/C_2^2\right)$, for some $C_1, C_2 > 0$, then there exists a constant $M_2 > 0$ which depends only on $C_1$, such that

$$E(X) \leq M_2 C_2.$$ 

A.2 Technical results

Lemma A.1. Let $\Psi_\alpha$ be the ERM rule on the tail region of level $1 - \alpha$ defined in (2.2). Given a dataset $D_n = (O_1, O_2, \ldots, O_n) \in \mathcal{X}^n$ and a sequence of mask $V_{1:K}$ it holds that

$$\hat{R}_\alpha(\Psi_\alpha(S_n), S_n) \leq \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}).$$

In other words the CV risk estimate of the ERM rule cannot be less than the empirical risk evaluated on the full dataset.

Proof. The argument for $\alpha \neq 1$ is the same as the one for $\alpha = 1$ (standard ERM) which may be found in Kearns and Ron 1999. We reproduce it for the sake of completeness. By definition of $\Psi_\alpha(S_n)$, one has

$$\forall j \in [1, n], \hat{R}_\alpha(\Psi_\alpha(T_j), S_n) \geq \hat{R}_\alpha(\Psi_\alpha(S_n), S_n).$$

Since $\hat{R}_\alpha(g, S_n) = \frac{1}{n} \left(n_V \hat{R}_\alpha(g, V_j) + n_T \hat{R}_\alpha(g, T_j)\right)$, for $g \in \mathcal{G}$ it follows that

$$\frac{1}{n} \left(n_V \hat{R}_\alpha(\Psi_\alpha(T_j), V_j) + n_T \hat{R}_\alpha(\Psi_\alpha(T_j), T_j)\right) \geq \frac{1}{n} \left(n_V \hat{R}_\alpha(\Psi_\alpha(S_n), V_j) + n_T \hat{R}_\alpha(\Psi_\alpha(S_n), T_j)\right).$$

Since $\Psi_\alpha(T_j)$ minimizes the training error on the $j$’th train set $T_j$, in particular we have

$$\hat{R}_\alpha(\Psi_\alpha(S_n), T_j) \geq \hat{R}_\alpha(\Psi_\alpha(T_j), T_j),$$

hence

$$\hat{R}_\alpha(\Psi_\alpha(S_n), V_j) \leq \hat{R}_\alpha(\Psi_\alpha(T_j), V_j), \forall j \in [1, K]. \quad (A.1)$$

In addition the average empirical risk of $\Psi_\alpha(S_n)$ is equal to its empirical risk on the full dataset, indeed

$$\frac{1}{K} \left(\sum_{j=1}^K \hat{R}_\alpha(\Psi_\alpha(S_n), V_j)\right) = \frac{1}{Kn_V} \left(\sum_{j=1}^K \sum_{i \in V_j} c(\Psi_\alpha(S_n), O_i) \mathbb{1}\left\{\|X_i\| > \|X_{(\alpha n_i)}\|\right\}\right)$$

$$= \frac{1}{Kn_V} \left(\sum_{j=1}^K \sum_{i=1}^n c(\Psi_\alpha(S_n), O_i) \mathbb{1}\{i \in V_j\} \mathbb{1}\{\|X_i\| > \|X_{(\alpha n_i)}\|\}\right)$$

$$= \frac{1}{Kn_V} \left(\sum_{i=1}^n c(\Psi_\alpha(S_n), O_i) \mathbb{1}\{\|X_i\| > \|X_{(\alpha n_i)}\|\}\right) \sum_{j=1}^K \mathbb{1}\{i \in V_j\}$$

(By lemma 2.1) $= \hat{R}_\alpha(\Psi_\alpha(S_n)).$
Thus by averaging inequality A.1, we get
\[ \hat{R}_\alpha(\Psi_\alpha(S_n), S_n) \leq \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}). \]

The following lemma is used in the proof of our second main result concerning l.p.o. risk estimation, see inequality (4.2). It is a generalization of Markov inequality that is particularly useful for cross-validation estimates. Our proof shares similarities with the proof of Theorem 4.1 in Kearns and Ron 1999 formulated under general algorithmic stability assumptions.

**Lemma A.2.** In the setting of Theorem 3.1, we have
\[
P(\hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_{CV,\alpha}(\Psi_\alpha, V_{1:K}) \geq t) \leq \frac{E(D_{t_\alpha} + \text{Bias} + |\hat{R}_\alpha(\Psi_\alpha(S_n), S_n) - R_\alpha(\Psi_\alpha(S_n))|)}{t},
\]
where Bias (resp. $D_{t_\alpha}$) is defined by equation 3.7 (resp 3.5).

**Proof.** Set
\[
\hat{R}_{CV,\alpha} = \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}), \quad R_{CV,\alpha} = R_{CV,\alpha}(\Psi_\alpha, V_{1:K}), \quad \hat{R}_\alpha = \hat{R}_\alpha(\Psi_\alpha(S_n), S_n), \quad R_\alpha = R_\alpha(\Psi_\alpha(S_n)).
\]
For any integrable real valued random variable $W$, and any $t > 0$ write $E[W] = P(W \geq t) E[W | W \geq t] + E[W 1\{W < t\}]$. Reorganising, we obtain the following generalized Markov inequality,
\[
P(W > t) = \frac{E(W) - E(W 1\{W < t\})}{E[W | W \geq t]} \leq \frac{E(W) - E(W 1\{W < t\})}{t}.
\]
Letting $W = \hat{R}_{CV,\alpha} - R_{CV,\alpha}$ we obtain
\[
P(\hat{R}_{CV,\alpha} - R_{CV,\alpha} \geq t) = \frac{E(\hat{R}_{CV,\alpha} - R_{CV,\alpha}) - E[(\hat{R}_{CV,\alpha} - R_{CV,\alpha}) 1\{\hat{R}_{CV,\alpha} - R_{CV,\alpha} \leq t\}]}{t} \quad (A.2)
\]
Using the fact that $E(\hat{R}_{CV,\alpha} - R_{CV,\alpha}) = 0$ and that $D_{t_\alpha} = |\hat{R}_{CV,\alpha} - \hat{R}_\alpha|$, one gets
\[
E(\hat{R}_{CV,\alpha} - R_{CV,\alpha}) = E(\hat{R}_{CV,\alpha} - \hat{R}_{\alpha}) \leq E(D_{t_\alpha}). \quad (A.3)
\]
Now using lemma A.1 write
\[
E[(R_{CV,\alpha} - \hat{R}_{CV,\alpha}) 1\{R_{CV,\alpha} - \hat{R}_{CV,\alpha} \leq t\}] \leq E[(R_{CV,\alpha} - \hat{R}_\alpha) 1\{R_{CV,\alpha} - \hat{R}_{CV,\alpha} \leq t\}]
\]
\[
\leq E[(R_{CV,\alpha} - \hat{R}_\alpha) 1\{R_{CV,\alpha} - \hat{R}_{CV,\alpha} \leq t\}]
\]
\[
\leq E[R_{CV,\alpha} - \hat{R}_\alpha] + E[|\hat{R}_{\alpha} - \hat{R}_\alpha|]
\]
\[
= E[\text{Bias}] + E[|\hat{R}_\alpha - \hat{R}_\alpha|]. \quad (A.4)
\]
The last line follows from the definition of Bias in (3.7). Combining inequality (A.2) with equations (A.3) and (A.4) yields
\[
P(\hat{R}_{CV,\alpha} - R_{CV,\alpha} \geq t) \leq \frac{E(D_{ta} + \text{Bias} + |\hat{R}_\alpha - R_\alpha|)}{t},
\]
which concludes the proof. \(\square\)

To conclude this section, we extend Theorem 10 in Goix et al. 2015 bounding the supremum deviations of the empirical measure on low probability regions, to handle the case of any cost function \(c\) absolutely bounded by one.

**Lemma A.3.** Recall the definitions of the risk \(R_\alpha\) and its empirical version \(\hat{R}_\alpha\) given in Section 2 and introduce the (random) supremum deviations
\[
Z' = \sup_{g \in G} |\hat{R}_\alpha(g, S_n) - R_\alpha(g)|.
\]
If \(G\) is a family of classifiers with finite VC-dimension and \(c\) a bounded cost function with \(\sup_{g,o} |c(g,o)| \leq 1\), then, the following Bernstein-type inequality holds,
\[
P(Z' - Q(n, \alpha) \geq t) \leq 3 \exp\left(\frac{-n\alpha t^2}{2(4 + t/3)}\right),
\]
where \(Q(n, \alpha) = B(n, \alpha) + \frac{1}{n\alpha}\) and \(B\) is defined by
\[
B(n, \alpha) = \frac{M \sqrt{V_G}}{\sqrt{\alpha n}} \quad (A.5)
\]
and \(M\) is a universal constant.

**Proof.** Write \(Z' \leq Z_1 + Z_2\) with :
\[
Z_1 = \sup_{g \in G} |\hat{R}_\alpha(g, S_n) - \hat{R}_\alpha(g, S_n)|,
\]
\[
Z_2 = \sup_{g \in G} |\hat{R}_\alpha(g, S_n) - R_\alpha(g)|.
\]
Concerning \(Z_2\), applying Corollary 5.1 with \(K = 1\) , \(V_1 = S_n\) yields
\[
P(Z_2 - B(n, \alpha) \geq t) \leq \exp\left(\frac{-n\alpha t^2}{2(4 + t/3)}\right). \quad (A.6)
\]
We now focus on \(Z_1\). Define
\[
u_i = \left|1\{\|X_i\| > \|X_{\lfloor \alpha n \rfloor}\}\right| - \frac{1}{n}\left|1\{\|X\| \geq t_\alpha\}\right|
\]
and notice that \(Z_1 \leq \frac{1}{n\alpha} \sum_{i=1}^n u_i\). It is known (see for instance the bound for the term \(A\) in Jalalzai et al. 2018, page 12) that
\[
\frac{1}{n\alpha} \sum_{i=1}^n u_i \leq \frac{1}{\alpha} \left|\frac{1}{n} \sum_{i=1}^n 1\{\|X\| \geq t_\alpha\} - \frac{1}{\alpha}\right| + \frac{1}{n\alpha}.
\]
Now, by noticing that $\text{Var}(\mathbb{1}\{\|X\| \geq t\alpha\}) \leq \alpha$ and using Bernstein’s inequality, we get
\[
P\left(\left|\frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\{\|X\| \geq t\alpha\} - \alpha\right| \geq t\right) \leq 2 \exp\left(\frac{-nt^2}{2(\alpha + t/3)}\right) \leq 2 \exp\left(\frac{-nt^2}{2(4\alpha + t/3)}\right).
\]

Finally, dividing by $\alpha$, we get
\[
P\left(\left|\frac{1}{\alpha} \sum_{i=1}^{n} \frac{1}{n} \mathbb{1}\{\|X\| \geq t\alpha\} - \frac{1}{\alpha} \right| \geq t\right) \leq 2 \exp\left(\frac{-n\alpha t^2}{2(4 + t/3)}\right).
\]

Therefore we finally obtain
\[
P\left(\frac{1}{\alpha} \sum_{i=1}^{n} u_i - \frac{1}{n\alpha} \geq t\right) \leq 2 \exp\left(\frac{-n\alpha t^2}{2(4 + t/3)}\right). \quad (A.7)
\]

The result follows using $Z' \leq Z_1 + Z_2$ and $Z_1 \leq \frac{1}{n\alpha} \sum_{i=1}^{n} u_i$. \hfill \square

Appendix B  Detailed proofs of the main results

B.1 Proof of Lemma 2.1

Since the leave-one-out is a special case of $K$-fold with $K = n$ (or leave-$p$-out with $p = 1$) it suffices to prove the statement concerning the cases of the leave-$p$-out and the $K$-fold.

$K$-Fold. For this procedure, the sequence of masks is a partition of $[1, n]$:
\[
\bigcup_{j=1}^{K} V_j = [1, n] \text{ and } V_j \cap V_k = \emptyset, \; \forall j \neq k \in [1, K]. \quad (B.1)
\]

Under the assumption that $K$ divides $n$, the condition $\text{card}(V_j) = n/K := n_V$ for all the validation sets $V_j$ holds, as stipulated in (2.4). Thus we have
\[
n = \sum_{j=1}^{K} \text{card}(V_j) = Kn_V. \quad (B.2)
\]

Furthermore, under (B.1), any index $l \in [1, n]$ belongs to a unique validation test $V_j$ and to all the train sets $T_j = V_j^c$ with $j \neq j'$. Hence, we both have
\[
\begin{cases}
\sum_{j=1}^{K} \mathbb{1}\{l \in T_j\} = K - 1, \quad \text{and} \\
\sum_{j=1}^{K} \mathbb{1}\{l \in V_j\} = 1.
\end{cases}
\]

Using (B.2) 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 sequence of validation sets is the family of all subsamples \( V_j \) of \( D_n \) of size \( \text{card}(V_j) = p \), thus \( K = \binom{n}{p} \). On the other hand, any index \( l \in [1, n] \) belongs to \( \binom{n-1}{p-1} \) validation sets. Indeed constructing a \( V_j \) such as \( l \in V_j \) is equivalent to first picking \( l \) and then choosing \( p-1 \) elements from \([1, n] \setminus \{l\}\). Hence we have

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

Using the identity \( n \binom{n-1}{p-1} = p \binom{n}{p} \) we obtain

\[
\frac{1}{KnV} \sum_{j=1}^{K} 1\{l \in V_j\} = \frac{1}{p} \binom{n}{p} \sum_{j=1}^{K} 1\{l \in V_j\} = 1/n,
\]

A similar argument applies to the sequence \( T_{1:K} \), which completes the proof.

**B.2 Proof of Lemma 5.1**

We introduce for convenience the rescaled variable \( Z_\alpha = \alpha Z \) where \( Z \) defined in (5.1) is the average of the supremum deviations of the (pseudo)-empirical risk \( \tilde{R}_\alpha \), see (3.1), over the validation sets \( V_j \). Then \( Z_\alpha \) may be written as

\[
Z_\alpha = \alpha \frac{1}{K} \sum_{j=1}^{K} \left[ \frac{1}{nV} \sup_{g \in G} \left| \sum_{i \in V_j(l)} c(g, O_i) \mathbb{1}_\alpha(X_i) - \mathbb{E}[c(g, O) \mathbb{1}_\alpha(X)] \right| \right],
\]

where we use the shorthand notation \( \mathbb{1}_\alpha(X) = I\{\|X\| \geq t_\alpha\} \). We derive an upper bound on \( P(Z_\alpha - \mathbb{E}(Z_\alpha) > t) \) using Proposition A.1. Namely we show that the maximum deviations term \( D \) and \( \sigma^2 \) from the latter statement are respectively bounded by \( D \leq 1/n \) and \( \sigma^2 \leq 4a/n \). To do so we compute explicitly the five quantities defined in the statement of Proposition A.1 in our particular context.

1. The conditional expectations \( f_i \) from Proposition A.1 are (recall that \( o_i = (x_i, y_i) \)),

\[
f_i(o_1, o_2, \ldots, o_l)
= \mathbb{E}(Z_\alpha \mid O_1 = o_1, O_2 = o_2, \ldots, O_l = o_l)
= \frac{1}{KnV} \sum_{j=1}^{K} \mathbb{E} \left[ \sup_{g \in G} \left| \sum_{i \in V_j} c(g, o_i) \mathbb{1}_\alpha(X_i) + \sum_{i \in V_j \setminus V_{j,l}} c(g, O_i) \mathbb{1}_\alpha(X_i) - \mathbb{E}[c(g, O) \mathbb{1}_\alpha(X)] \right| \right]
= \frac{1}{KnV} \sum_{j=1}^{K} \mathbb{E} \left[ \sup_{g \in G} |h_{j,l,g}| \right],
\]
where \( V_{j,l} = V_j \cap [1,l] \) are the mask’s indices which belong to the interval \([1,l]\), and
\[
\begin{align*}
    h_{j,l,g} = \sum_{i \in V_{j,l}} c(g, o_i) \mathbb{1}_a(x_i) + \sum_{i \in V_j \setminus V_{j,l}} c(g, O_i) \mathbb{1}_a(X_i) - \mathbb{E}[c(g, O) \mathbb{1}_a(X)].
\end{align*}
\]

2. Recall the definition of the positive deviations \( \Delta_l \),
\[
\Delta_l(o_1, o_2, \ldots, o_{l-1}, o_l) = f_l(o_1, o_2, \ldots, o_{l-1}, o_l) - f_{l-1}(o_1, o_2, \ldots, o_{l-1}).
\]
In view of the expression for \( f_l \) from step 1, we may thus write
\[
\Delta_l(o_1,l) = \frac{1}{KnV} \sum_{j=1}^{K} \mathbb{E} \left[ \sup_{g \in \mathcal{G}} \left| h_{j,l,g} \right| - \sup_{g \in \mathcal{G}} \left| h_{j,l-1,g} \right| \right].
\]
Now, notice that \( V_{j,l} = V_{j,l-1} \) if \( l \notin V_j \) and \( V_{j,l} = V_{j,l-1} \cup \{l\} \) otherwise. Hence
\[
h_{j,l,g} - h_{j,l-1,g} = \mathbb{1}\{l \in V_j\} \left( c(g, o_l) \mathbb{1}_a(x_l) - c(g, O_l) \mathbb{1}_a(X_l) \right).
\]
Using the fact that, for any functions \( f, g \), it holds that \( |\sup f - \sup g| \leq \sup |f-g| \),
we obtain
\[
|\Delta_l(o_1,l)| \leq \frac{1}{KnV} \sum_{j=1}^{K} \mathbb{E} \left[ \sup_{g \in \mathcal{G}} \left| c(g, o_l) \mathbb{1}_a(x_l) - c(g, O_l) \mathbb{1}_a(X_l) \right| \right] \leq 1
\]
and deduce that
\[
|\Delta_l(o_1,l)| \leq \frac{1}{KnV} \sum_{j=1}^{K} \mathbb{1}\{l \in V_j\} \leq \frac{1}{n} \quad \text{(by (2.5))}.
\]

3. The maximum positive deviation is defined by \( D := \max_{l=1,\ldots,n} \sup_{o_1,\ldots,o_{l-1} \in \mathcal{X}} \sup_{o \in \mathcal{X}} \Delta_l(o_1, \ldots, o_{l-1}, o). \)
From the previous step, we immediately obtain
\[
D \leq 1/n.
\]

4. Let \( O' = (X', Y') \) be an independent copy of \( O = (X, Y) \) and let \( o_{1:l} = (o_1, o_2, \ldots, o_l) \). Recall the conditional variance term from the statement of Proposition A.1, \( \sigma_l^2(o_{1:l-1}) := \text{Var}[\Delta_l(O_1, O_2, \ldots, O_{l-1}, O') \mid O_1 = o_1, O_2 = o_2, \ldots, O_{l-1} = o_{l-1}] \). Then \( \sigma_l^2 \) may be upper bounded as follows,
\[
\sigma_l^2(o_{1:l-1}) \leq \mathbb{E} \left[ \Delta_l(O_1, O_2, \ldots, O_{l-1}, O')^2 \mid O_1 = o_1, O_2 = o_2, \ldots, O_{l-1} = o_{l-1} \right] = \mathbb{E} \left[ \Delta_l(o_1, o_2, \ldots, o_{l-1}, O')^2 \right].
\]
Now using (B.3), write

$$\sigma_l^2 \leq \frac{1}{(KnV)^2} \mathbb{E} \left[ \left( \sum_{j=1}^K \mathbbm{1}\{l \in V_j\} \mathbb{E} \left[ \sup_{g \in G} |c(g, O') \mathbbm{1}_a(X') - c(g, O_l) \mathbbm{1}_a(X_l)| \mid X' \right] \right)^2 \right]$$

$$\left( |c| \leq 1 \right) \leq \frac{1}{KnV} \mathbb{E} \left[ \left( \sum_{j=1}^K \mathbbm{1}\{l \in V_j\} \mathbb{E} \left[ \sup_{g \in G} \mathbbm{1}_a(X') + \mathbbm{1}_a(X_l) \mid X' \right] \right)^2 \right]$$

$$= \frac{1}{KnV} \mathbb{E} \left[ \left( \sum_{j=1}^K \mathbbm{1}\{l \in V_j\} \left( \mathbbm{1}_a(X') + \alpha \right) \right)^2 \right]$$

$$\leq \mathbb{E} \left[ (\mathbbm{1}_a(X') + \alpha)^2 \right] \left( \frac{1}{KnV} \sum_{j=1}^K \mathbbm{1}\{l \in V_j\} \right)^2$$

$$= (\alpha^2 + 3\alpha) \left( \frac{1}{KnV} \sum_{j=1}^K \mathbbm{1}\{l \in V_j\} \right)^2$$

(by (2.5)) = \frac{\alpha^2 + 3\alpha}{n^2}

(\alpha \leq 1 \leq \frac{4\alpha}{n^2}.

5. Finally get \(\sigma^2 = \sum_{l=1}^n \sup_{\alpha_{l-1}} \sigma_l^2(\alpha_{l-1}) \leq \frac{4\alpha}{n^2}.

At this stage, applying proposition A.1 gives

$$\mathbb{P}(Z_\alpha - \mathbb{E}[Z_\alpha] > t) \leq \exp \left\{ \frac{-nt^2}{2(4\alpha + t/3)} \right\}.$$ 

Therefore for \(Z = Z_\alpha/\alpha\) one obtains

$$\mathbb{P}(Z - \mathbb{E}[Z] > t) \leq \exp \left\{ \frac{-n\alpha t^2}{2(4 + t/3)} \right\}.$$ 

### B.3 Proof of lemma 5.2

Notice first that, since the observations are i.i.d.,

$$\mathbb{E} \left[ \frac{1}{K} \sum_{j=1}^K \sup_{g \in G} \left| \tilde{R}_\alpha(g, V_j) - R_\alpha(g) \right| \right] = \mathbb{E} \left[ \sup_{g \in G} \left| \tilde{R}_\alpha(g, V_1) - R_\alpha(g) \right| \right].$$

That is, \(\mathbb{E}(Z) = \mathbb{E}(Z_{V_1})\), where for a subset of indices \(S = \{1, \ldots, n_S\}\), we denote

$$Z_S = \sup_{g \in G} \left| \tilde{R}_\alpha(g, S) - R_\alpha(g) \right|.$$
In order to bound $E[Z_S]$ defined above, we follow the same steps as in the proof of Lemma 14 in Goix et al. 2015, where most arguments also hold true for a bounded VC class of cost functions. We use the symmetrization technique. Consider Rademacher random variables $\mathcal{E} = (\epsilon_1, \epsilon_2, \ldots, \epsilon_n)$ taking values in $\{-1, 1\}$ and introduce the randomized process

$$Z_{\mathcal{E}} = \sup_{g \in \mathcal{G}} \left| \frac{1}{\alpha n_S} \sum_{i=1}^{n_S} \epsilon_i c(g, O_i) \mathbf{1}\{\|X_i\| > t_\alpha\} \right|.$$ 

It can be shown using the same classical steps as in the proof of Lemma 13 in Goix et al. 2015 that

$$E(Z_S) \leq 2E(Z_{\mathcal{E}}).$$

The key argument to the proceed is to condition the above expectation upon the number of indices $i$ such that $\|X_i\| > t_\alpha$. Introduce the random variable $O_\alpha$, which has the same distribution as $(O_\|X\| \geq t_\alpha)$ and notice that

$$\sum_{i=1}^{n_S} \epsilon_i c(g, O_i) \mathbf{1}\{\|X_i\| > t_\alpha\} \sim \sum_{i=1}^{N} \epsilon_i c(g, O_{i,\alpha}),$$

where $N$ has a Binomial distribution $B(n_S, \alpha)$. Equipped with these notations

$$E(Z_{\mathcal{E}}) = E(\phi(N)),$$

where $\phi(N) = E \sup_{g \in \mathcal{G}} \left| \frac{1}{\alpha n_S} \sum_{i=1}^{N} \epsilon_i c(g, O_{i,\alpha}) \right| = \frac{N}{\alpha n_S} E \sup_{g \in \mathcal{G}} \left| \sum_{i=1}^{N} \epsilon_i c(g, O_{i,\alpha}) \right|.$$

Then by some classical Rademacher complexity arguments for finite VC-classes (see e.g. Giné and Guillou 2001, Proposition 2.1),

$$E \sup_{g \in \mathcal{G}} \left| \frac{1}{N} \sum_{i=1}^{N} \epsilon_i c(g, O_{i,\alpha}) \right| \leq M_1' \sqrt{\frac{V_{\mathcal{G}}}{N}} + \frac{M_2' V_{\mathcal{G}}}{N} \leq M' \sqrt{\frac{V_{\mathcal{G}}}{N}},$$

for some universal constant $M' > 0$, whence

$$\phi(N) \leq \frac{N}{\alpha n_S} M' \sqrt{\frac{V_{\mathcal{G}}}{n_S}} \leq \frac{M' \sqrt{V_{\mathcal{G}} n_S}}{\alpha n_S}.$$

By concavity we have $E(\sqrt{N}) \leq \sqrt{E(N)} = \alpha n_S$, and we obtain

$$E(Z_S) \leq 2E(Z_{\mathcal{E}}) \leq 2M' \sqrt{\frac{V_{\mathcal{G}}}{n_S}}.$$

The result follows with $n_S = n_V$.

**B.4 Detailed proof of Theorem 3.1**

In view of the argument following the statement, we derive probability upper bounds for the three terms $D_{t_\alpha}, D_{cv}$ and Bias defined in equations (3.5, 3.6, 3.7).
**Probability bound for** $D_{t\alpha}$ (see (3.5)). Using the fact that the cost function verifies $0 \leq c \leq 1$, write

$$D_{t\alpha} = |\tilde{R}_{CV,\alpha}(\Psi_{\alpha}, V_{1:K}) - \tilde{R}_{CV,\alpha}(\Psi_{\alpha}, V_{1:K})| \leq U,$$

where $U = \frac{1}{Kn_{V\alpha}} \sum_{j=1}^{K} \sum_{i \in V_j} u_i$ and (we recall that)

$$u_i = \mathbb{1}\{\|X_i\| > \|X_{(\lfloor n\alpha\rfloor)}\|\} - \mathbb{1}\{\|X_i\| \geq t_{\alpha}\}.$$

Now notice that

$$U = \frac{1}{Kn_{V\alpha}} \sum_{j=1}^{K} \sum_{i=1}^{n} u_i \mathbb{1}\{i \in V_j\}$$

$$= \frac{1}{Kn_{V\alpha}} \sum_{i=1}^{n} u_i \sum_{j=1}^{V} \mathbb{1}\{i \in V_j\}$$

$$= \frac{1}{n\alpha} \sum_{i=1}^{n} u_i.$$

The last line follows from Assumption 2. Hence, using (A.7), we obtain

$$P(D_{t\alpha} - 1/n\alpha \geq t) \leq 2 \exp\left(\frac{-n\alpha t^2}{2(4 + t/3)}\right). \quad (B.4)$$

**Probability bound for** $D_{CV}$ (see 3.6)). First, notice that

$$C_{CV} = \frac{1}{K} \sum_{j=1}^{K} |\tilde{R}_{\alpha}(\Psi_{\alpha}(T_j), V_j) - \tilde{R}_{\alpha}(\Psi_{\alpha}(T_j))|$$

$$\leq \frac{1}{K} \sum_{j=1}^{K} \sup_{g \in \mathcal{G}} |\tilde{R}_{\alpha}(g, V_j) - R_{\alpha}|.$$

Using Corollary 5.1 with

$$Z = \frac{1}{K} \sum_{j=1}^{K} \sup_{g \in \mathcal{G}} |\tilde{R}_{\alpha}(g, V_j) - R_{\alpha}(g)|,$$

one obtains the inequality

$$P(D_{CV} - B(n_V, \alpha) \geq t) \leq \exp\left(\frac{-n\alpha t^2}{2(4 + t/3)}\right), \quad (B.5)$$

with

$$B(n_V, \alpha) = \frac{M \sqrt{V_\alpha}}{\sqrt{nV}},$$

for some universal constant $M > 0$. 

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Probability bounds for Bias (see (3.7)). We write

$$\text{Bias} = \frac{1}{K} \left| \sum_{j=1}^{K} \left( R_\alpha(\Psi_\alpha(T_j)) - R_\alpha(\Psi_\alpha(S_n)) \right) \right| \leq C_1 + C_2, \quad (B.6)$$

with

$$C_1 = \frac{1}{K} \left| \sum_{j=1}^{K} \left( R_\alpha(\Psi_\alpha(T_j)) - \hat{R}_\alpha(\Psi_\alpha(T_j), T_j) + \hat{R}_\alpha(\Psi_\alpha(T_j), T_j) - R_\ast \right) \right|,$$

$$C_2 = \left| R_\ast - \hat{R}_\alpha(\Psi_\alpha(S_n), S_n) + \hat{R}_\alpha(\Psi_\alpha(S_n), S_n) - R_\alpha(\Psi_\alpha(S_n)) \right|$$

and

$$R_\ast = \inf_{g \in G} R_\alpha(g).$$

Using the fact that $\hat{R}_\alpha(\Psi_\alpha(T_j), T_j) = \inf_{g \in G} \hat{R}_\alpha(g, T_j)$ (Assumption 1) and for any real functions $h$ and $f$, $|\inf h - \inf f| \leq \sup|h - f|$, write

$$\frac{1}{K} \left| \sum_{j=1}^{K} \left( \hat{R}_\alpha(\Psi_\alpha(T_j), T_j) - R_\ast \right) \right| = \frac{1}{K} \left| \sum_{j=1}^{K} \inf_{g \in G} \hat{R}_\alpha(g, T_j) - \inf_{g \in G} R_\alpha(g) \right| \leq \frac{1}{K} \sum_{j=1}^{K} \left| \inf_{g \in G} \hat{R}_\alpha(g, T_j) - \inf_{g \in G} R_\alpha(g) \right| \leq \frac{1}{K} \sum_{j=1}^{K} \sup_{g \in G} |\hat{R}_\alpha(g, T_j) - R_\alpha(g)|.$$

Then, by using the triangle inequality, deduce that

$$C_1 \leq 2 \frac{1}{K} \sum_{j=1}^{K} \sup_{g \in G} |\hat{R}_\alpha(g, T_j) - R_\alpha(g)| \leq Z_1 + Z_2, \quad (B.7)$$

with

$$Z_1 = 2 \frac{1}{K} \sum_{j=1}^{K} \sup_{g \in G} |\hat{R}_\alpha(g, T_j) - \hat{R}_\alpha(g, T_j)|,$$

$$Z_2 = 2 \frac{1}{K} \sum_{j=1}^{K} \sup_{g \in G} |\hat{R}_\alpha(g, T_j) - R_\alpha(g)|.$$

In order to bound $Z_2$ we use the fact that the statements of Lemmas 5.1, 5.2 and Corollary 5.1 still hold true if one substitutes the training sets $T_j$ for the validation sets $V_j$, and the training
size $n_T$ for $n_V$, as revealed by an inspection of the proofs, see Sections B.2 and B.3. The only difference between the two arguments is in steps 2 and 4 from the proof of Lemma 5.1 where we use the identity $\frac{1}{K} \sum_{j=1}^{K} \frac{1}{n} \{ l \in T_j \} = \frac{1}{n}$ from Lemma 2.1 instead of Identity (2.5). Thus we obtain, from the twin statement of Corollary 5.1,

$$
P(Z_2 - 2B(n_T, \alpha) \geq 2t) \leq 2 \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right), \quad (B.8)
$$

where $B(n, \alpha)$ is defined in (A.5).

Similarly the term $Z_1$ can be bounded following the same argument as in the first paragraph (Probability bound for $D_{n, \alpha}$) up to replacing $V_j$ with $T_j$ and $n_V$ with $n_T$, which yields

$$
P(Z_1 - \frac{2}{n_T \alpha} \geq 2t) \leq 4 \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right). \quad (B.9)
$$

Decomposition (B.7) combined with inequalities (B.8), (B.9) leads to

$$
P(C_1 - 2Q(n_T, \alpha) \geq 4t) \leq 6 \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right), \quad (B.10)
$$

with

$$
Q(n, \alpha) = B(n, \alpha) + \frac{1}{n\alpha} = \frac{M \sqrt{\sum_{g \in G} \alpha n}}{\sqrt{\alpha n}} + \frac{1}{n\alpha}. \quad (B.11)
$$

Using the same technique, one has

$$
C_2 \leq 2 \sup_{g \in \beta} |\hat{R}_\alpha(g, S_n) - R_\alpha(g)|.
$$

Then by Lemma A.3, we obtain

$$
P(C_2 - 2Q(n_T, \alpha) \geq 4t) \leq 6 \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right). \quad (B.12)
$$

Moreover, notice that we have

$$
\begin{align*}
4B(n_T, \alpha) &\geq 2B(n, \alpha) + 2B(n_T, \alpha), \\
\frac{4}{n_T \alpha} &\geq \frac{2}{n \alpha} + \frac{2}{n\alpha}.
\end{align*}
$$

Therefore we get

$$
4Q(n_T, \alpha) \geq 2Q(n, \alpha) + 2Q(n_T, \alpha). \quad (B.13)
$$

Combining equations (B.10), (B.12), (B.13) and decomposition (B.6) yields

$$
P(\text{Bias} - 4Q(n_T, \alpha) \geq 8t) \leq 12 \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right). \quad (B.14)
$$
Assembling terms. Using equations (B.4), (B.5), (B.14) and the decomposition (3.4), deduce the inequality

\[ \Pr \left( \left| \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_\alpha(\Psi_\alpha(S_n)) \right| - E_{CV}(n_T, n_V, \alpha) \geq 10t \right) \leq 15 \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right), \]

with

\[ E_{CV}(n_T, n_V, \alpha) = B(n_V, \alpha) + 4Q(n_T, \alpha) + \frac{1}{n_T \alpha}, \]

The last line follows, using the definitions of \( B \) (eq. A.5) and \( Q \) (eq. B.11).

By inverting inequality (B.15), one has, with probability \( 1 - 15\delta \),

\[ \left| \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_\alpha(\Psi_\alpha(S_n)) \right| \leq E_{CV}(n_T, n_V, \alpha) + \frac{20}{3n\alpha} \log \left( \frac{1}{\delta} \right) + 20 \sqrt{\frac{2}{n\alpha} \log \left( \frac{1}{\delta} \right)}, \]

which is the desired result.

B.5 Proof of Theorem 4.1

In view of the discussion following the statement of the theorem (namely the risk decomposition (4.1) and the Markov-type inequality (4.2)) and the bound for the term Bias obtained in (B.14), we only need to obtain bounds for the expectations \( E(D_{t_\alpha}) \), \( E(\text{Bias}) \), and \( E(|\hat{R}_\alpha(\Psi_\alpha(S_n), S_n) - R_\alpha(\Psi_\alpha(S_n))|) \). The proof will then be completed by combining together the different terms.

Bounding \( E(D_{t_\alpha}) \). By equation B.4, one has

\[ \Pr(D_{t_\alpha} - \frac{1}{n\alpha} \geq t) \leq \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right). \]

On the one hand, under Assumption 4 one has \( \Pr(D_{t_\alpha} - \frac{1}{n\alpha} \geq t) = 0 \) for \( t \geq 2 \). On the other hand, we have the trivial inequality,

\[ \forall t \leq 2, \ 2(4 + t/3) \leq 10. \]

Hence we can write, for \( t \geq 0 \),

\[ \Pr(D_{t_\alpha} - \frac{1}{n\alpha} \geq t) \leq \exp \left( \frac{-n\alpha t^2}{10} \right). \]

Therefore by lemma A.2, we get

\[ E(D_{t_\alpha}) \leq \frac{1}{n\alpha} + \frac{M_1}{\sqrt{n\alpha}} \]

\[ \leq \frac{1}{n_T \alpha} + \frac{M_1}{\sqrt{n_T \alpha}}, \]

for some universal constant \( M_1 > 0 \).
Bounding $\mathbb{E}(\text{Bias})$. Using equation (B.14) and reasoning as in the previous paragraph leads to

$$
\mathbb{E}(\text{Bias}) \leq 4Q(nT, \alpha) + \frac{M_2}{\sqrt{nT\alpha}}, \quad (B.18)
$$

where $Q(n, \alpha)$ is defined by (B.11) and $M_2 > 0$ is a universal constant, independent of $G, n$ and $\alpha$.

Bounding $\mathbb{E}(|\hat{\mathcal{R}}_\alpha(\Psi_\alpha(S), S_n) - \mathcal{R}_\alpha(\Psi_\alpha(S))|)$. By lemma A.3 we obtain

$$
\mathbb{P}(\hat{\mathcal{R}}_\alpha(\Psi_\alpha(S), S_n) - \mathcal{R}_\alpha(\Psi_\alpha(S))| - Q(n, \alpha) \geq 2t) \leq 3 \exp\left(\frac{-n\alpha t^2}{2(4 + t/3)}\right). \quad (B.19)
$$

Then we get

$$
\mathbb{E}(\hat{\mathcal{R}}_\alpha(\Psi_\alpha(S), S_n) - \mathcal{R}_\alpha(\Psi_\alpha(S))) \leq Q(n, \alpha) + \frac{M_3}{\sqrt{n\alpha}}, \quad (B.20)
$$

for some universal constant $M_3 > 0$.

Combining equations (B.17), (B.18), (B.20) with Lemma A.2 gives

$$
\mathbb{P}(\hat{\mathcal{R}}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - \mathcal{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) \geq t) \leq \frac{5Q(nT, \alpha) + \frac{M_4}{\sqrt{nT\alpha}}}{t} + \left(\frac{1}{nT\alpha}\right), \quad (B.21)
$$

where $M_4 = M_1 + M_2 + M_3$. The next step is to derive a probability bound for $\mathcal{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - \hat{\mathcal{R}}_{CV,\alpha}(\Psi_\alpha, V_{1:K})$. We have

$$
\mathbb{P}(\mathcal{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - \hat{\mathcal{R}}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - 5Q(nT, \alpha) \geq 10t)
\leq \mathbb{P}(\mathcal{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - \hat{\mathcal{R}}_\alpha(\Psi_\alpha(S), S_n) - 5Q(nT, \alpha) \geq 10t)
\leq \mathbb{P}(\mathcal{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - \mathcal{R}_\alpha(\Psi_\alpha(S)) - 4Q(nT, \alpha) \geq 8t)
+ \mathbb{P}(\mathcal{R}_\alpha(\Psi_\alpha(S)) - \hat{\mathcal{R}}_\alpha(\Psi_\alpha(S), S_n) - Q(nT, \alpha) \geq 2t)
\leq \mathbb{P}(\hat{\mathcal{R}}_\alpha(\Psi_\alpha(S), S_n)) - \mathcal{R}_\alpha(\Psi_\alpha(S))| - Q(nT, \alpha) \geq 2t)
+ \mathbb{P}(\text{Bias} - 4Q(nT, \alpha) \geq 8t)
\leq 15 \exp\left(\frac{-n\alpha t^2}{2(4 + t/3)}\right). \quad (B.22)
$$

The first inequality follows from the fact that $\hat{\mathcal{R}}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) \geq \hat{\mathcal{R}}_\alpha(\Psi_\alpha(S), S_n)$ (lemma A.1). The second inequality is obtained by a union bound. The third inequality follows from the definition of Bias (eq. 3.7). Combining (B.21) and (B.22) and that

$$
\mathbb{P}(|X| \geq 10t) \leq \mathbb{P}(X \geq 10t) + \mathbb{P}(-X \geq 10t) \leq \mathbb{P}(X \geq t) + \mathbb{P}(-X \geq 10t),
$$

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leads to

\[
P \left( \left| \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_{CV,\alpha}(\Psi_\alpha, V_{1:K}) \right| - 5Q(n_T, \alpha) \geq 10t \right) \\
\leq \frac{5Q(n_T, \alpha)}{t} + \frac{M_4/\sqrt{n_T \alpha}}{t} + \frac{(1/n_T \alpha)}{t} + 15 \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right). \quad (B.23)
\]

Finally, using (4.1), we get

\[
P \left( \left| \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_\alpha(\Psi_\alpha(S_n)) \right| - 9Q(n_T, \alpha) \geq 18t \right)
\leq P(\text{Bias} - 4Q(n_T, \alpha) \geq 8t) + P \left( \left| \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_{CV,\alpha}(\Psi_\alpha, V_{1:K}) \right| - 5Q(n_T, \alpha) \geq 10t \right)
\leq \frac{Q(n_T, \alpha)}{t} + \frac{(M_4/\sqrt{n_T \alpha})}{t} + 18 \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right). \quad (B.24)
\]

The last line follows from (B.14) and (B.23). Since for any \( t \geq 2 \),

\[
P \left( \left| \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_\alpha(\Psi_\alpha(S_n)) \right| - 9Q(n_T, \alpha) \geq 18t \right) = 0
\]

we can restrict our attention to the case \( t \leq 2 \), for which we have

\[
27 \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right) \leq 27 \exp \left( \frac{-n\alpha t^2}{10} \right).
\]

Using that \( \exp(-x) \leq \frac{1}{x} \) for \( x \geq 0 \), we deduce that

\[
27 \exp \left( \frac{-n\alpha t^2}{2(4 + t/3)} \right) \leq \frac{270}{n\alpha t^2}.
\]

Using the latter inequality and inverting (B.24), we get that with probability \( 1 - 18\delta \),

\[
\left| \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_\alpha(\Psi_\alpha(S_n)) \right| \leq 9Q(n_T, \alpha + \frac{5Q(n_T, \alpha)}{\delta/\sqrt{n_T \alpha}} + (1/n_T \alpha) + \sqrt{\frac{270}{n_T \alpha \delta}},
\]

Using the fact that \( \sqrt{\frac{t}{\delta}} \leq \frac{1}{\delta} \) (since \( \delta \leq 1 \)), the latter inequality becomes:

\[
\left| \hat{R}_{CV,\alpha}(\Psi_\alpha, V_{1:K}) - R_\alpha(\Psi_\alpha(S_n)) \right| \leq 9Q(n_T, \alpha + \frac{1}{\delta/\sqrt{n_T \alpha}}(5Q(n_T, \alpha) + M_5) + \frac{1}{\delta n_T \alpha},
\]

with \( M_5 = M_4 + \sqrt{270} \). Replacing \( Q \) with its expression (Equation B.11) gives the desired result.