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Risk Bounds for Embedded Variable Selection in Classification Trees

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Abstract

The problems of model and variable selections for classification trees are jointly considered. A penalized criterion is proposed which explicitly takes into account the number of variables, and a risk bound inequality is provided for the tree classifier minimizing this criterion. This penalized criterion is compared to the one used during the pruning step of the CART algorithm. It is shown that the two criteria are similar under some specific margin assumptions. In practice, the tuning parameter of the CART penalty has to be calibrated by hold-out. Simulation studies are performed which confirm that the hold-out procedure mimics the form of the proposed penalized criterion.

Keywords: Classification Tree, Variable Selection, Statistical Learning Theory

1 Introduction

Since the pioneering work of Breiman *et al.* [Breiman et al., 1984], classification trees have become a classical tool in machine learning. In particular, the Classification and Regression Tree (CART) algorithm is a well-established algorithm to build and prune tree predictors. This algorithm has been successfully applied in various fields, see for instance Bel et al. [2009], Chou et al. [1989], Dudoit et al. [2002], Wernecke et al. [1998]. A crucial step of the CART algorithm is the pruning process, in which a tree classifier \hat{f}_T is selected from a short list of classifiers based on trees pruned from a deep tree T_{max} . The penalized criterion proposed to select \hat{f}_T is of the form

$$P_n \hat{f}_T + \alpha_n \times |T| \quad , \quad (1)$$

where n is the number of observations, $P_n \hat{f}_T$ is the empirical risk of tree classifier \hat{f}_T , α_n is a tuning parameter (known to depend on n , see Gey and Nedelec [2005] for instance), and $|T|$ is the size of the tree, i.e. the number of leaves (terminal nodes) of T .

From a theoretical point of view, many works have investigated this pruning process. In the Gaussian or bounded regression context, this criterion was validated in Gey and Nedelec [2005] using model selection framework. Another validation was obtained in the classification framework in Nobel [2002]. More recently, a refined analysis of the pruning step was proposed in Gey [2010], where margin adaptive risk bounds were obtained in the binary classification context.

However, the results obtained so far are not completely satisfactory for at least two reasons. First, by considering the problem of performance assessment for tree classifiers only through the pruning step, one can only obtain theoretical guarantees conditionally to the construction of T_{max} . In this case, the performance of the candidate classifier \hat{f}_T is compared to the best performance that can be achieved by one of the classifiers built on the subtrees of T_{max} . The alternative point of view adopted here will be to compare the performance of a candidate tree classifier to the best performance that can be achieved by one of the classifiers built on *any* tree. Second, it is well-known that CART belongs to the embedded variable selection methods (Czekaj et al. [2008], Guyon and Elisseeff [2003], Lal et al. [2006]). A variable selection process is called embedded when it is included in the training step of the classification algorithm. Therefore the learning and variable selection processes cannot be separated. In CART, this inner selection process results from the recursive growing strategy of the tree: at each node, the “best” variable is selected among all for splitting. As a result, in many cases the maximal tree (and consequently all of its subtrees) only includes a small subset of the p initial variables. This embedded property is actually one of the main arguments for the use of CART to deal with large dimension data (see Breiman [2001], Dyer et al. [2007], Gey and Lebarbier [2008] for example). However, criterion (1) does not obviously depend on the total number of covariates p . This can be astonishing: in both the regression and classification frameworks, theoretical studies have shown that in the variable selection context, an extra term should be added to the penalty that is used when only one model is considered per dimension (Birgé and Massart [2001], Mary-Huard et al. [2007]) to obtain oracle-type inequalities. Since the collection of possible trees increases with p , p should play a crucial role in the regularization term.

Since parameter p does not explicitly appear in criterion (1), one can argue that p is hidden in the constant term α_n . This argument is verified from at least two penalties that can be exhibited from previous works:

- In Nobel [2002] (equation 4), the penalty term has the form

$$\begin{aligned} pen(|T|, n) &= C_1 \times \sqrt{\frac{|T|p \log n}{n}} \\ &= \sqrt{Cst \frac{p \log n}{n}} \times \sqrt{|T|} \\ &= \alpha(p, n) \sqrt{|T|} \ , \end{aligned}$$

- In Gey [2010] (Theorem 1), the penalty term is of order

$$\begin{aligned} pen(|T|, n) &\approx C_2 \times \frac{p \log(p)(1 + \log(n/\log(p)))}{n} \times |T| \\ &= \alpha(p, n) |T| \ , \end{aligned}$$

where C_1 and C_2 are known constants. While these two penalty functions depend on p , one can observe that their scaling order is much larger than the $\log(p)$ usually obtained in the variable selection context (Birgé and Massart [2001], Mary-Huard et al. [2007]).

The goal of the present paper is to decipher the exact impact of variable selection on tree classifier selection. First, this will be investigated from a theoretical point of view. To this purpose, we consider the model selection problem where the goal is to select a candidate

from all possible tree classifiers. The strategy consists in choosing the candidate minimizing a penalized criterion that depends on parameters p and n , and on the margin assumption made on the conditional distribution of the label. In this model selection context, we exhibit a penalization function where the variable selection process is explicitly taken into account, and provide performance guarantees for the candidate tree classifier through an upper bound of its risk. The impact of variable selection is then studied from a practical point of view. A simulation study is performed which shows that the proposed penalization function is the one that is implicitly used in the pruning step of the CART algorithm.

The paper is organized as follows. Section 2 presents the framework of binary classification and describes tree classifiers. The main theoretical contribution and the simulation study are presented in Section 3. Some discussion is developed in Section 4, and finally Section 5 gives the proofs of the results presented in Section 3.

2 Context

2.1 Classification framework

The considered classification framework is the following. Suppose one observes a sample $\{(X_1, Y_1), \dots, (X_n, Y_n)\}$ of n independent copies of the random variable (X, Y) , where the explanatory variable X takes values in a measurable space \mathcal{X} of dimension $p \geq 2$, and is associated with a label Y taking values in $\{0, 1\}$. Suppose moreover that each coordinate of \mathcal{X} is ordered. A classifier is then any function f mapping \mathcal{X} into $\{0, 1\}$. The quality of a classifier is measured by its misclassification rate

$$Pf := P(f(X) \neq Y) \quad , \quad (2)$$

where P denotes the joint distribution of (X, Y) . If the joint distribution of (X, Y) were known, the problem of finding an optimal classifier minimizing the misclassification rate would be easily solved by considering the Bayes classifier f^* defined for every $x \in \mathcal{X}$ by

$$f^*(x) = \mathbb{1}_{\eta(x) \geq 1/2} \quad , \quad (3)$$

where $\eta(x)$ is the conditional expectation of Y given $X = x$, that is

$$\eta(x) = P[Y = 1 \mid X = x] \quad . \quad (4)$$

As P is unknown, the goal is to construct from sample $\{(X_1, Y_1), \dots, (X_n, Y_n)\}$ a classifier \tilde{f} that is as close as possible to f^* in the following sense: since f^* minimizes the misclassification rate, \tilde{f} will be chosen in such a way that its misclassification rate is as close as possible to the misclassification rate of f^* , i.e. in such a way that the loss

$$l(f^*, \tilde{f}) = P(\tilde{f}(X) \neq Y) - P(f^*(X) \neq Y) \quad (5)$$

is as small as possible.

Many strategies or classification algorithms have been proposed to build \tilde{f} (see [Hastie et al. \[2001\]](#), [Boucheron et al. \[2005\]](#) for an overview). The quality of a strategy is measured by its risk

$$\mathbb{E}[l(f^*, \tilde{f})] \quad ,$$

where the expectation is taken with respect to the sample distribution. In the model selection framework, two strategies are usually considered:

- Empirical Risk Minimization: \tilde{f} is chosen as the minimizer of

$$P_n f := \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{f(X_i) \neq Y_i\}} \quad , \quad (6)$$

over all classifiers f belonging to a single class of classifiers,

- Structural Risk Minimization: \tilde{f} is chosen as the minimizer of the penalized empirical risk over a collection of classes.

2.2 Margin assumptions

It is now well known that without any assumption on the joint distribution P , the minimax convergence rate of the risk bound is of order $\mathcal{O}(1/\sqrt{n})$. It has also been shown that, under the overoptimistic zero-error assumption (that is $Y = \eta(X)$ almost surely, where η is defined by (4)), this minimax convergence rate is of order $\mathcal{O}(1/n)$ (see Vapnik [1998], Lugosi [2002] for example).

These two extreme cases can be modulated by so-called *margin assumptions* that make the link between the “global” pessimistic case (without any assumption on P) and the zero-error case (Koltchinskii [2006a,b], Mammen and Tsybakov [1999], Massart and Nédélec [2006], Massart [2007], Tsybakov [2004], Tsybakov and van de Geer [2005]).

In this paper, we consider the margin assumption proposed in Mammen and Tsybakov [1999]:

MA(1) There exist some constants $C > 0$ and $\kappa > 1$ such that, for all $t > 0$,

$$P(|2\eta(X) - 1| \leq t) \leq C t^{\frac{1}{\kappa-1}}, \quad (7)$$

Note that by taking $t = h \in]0, 1[$ and $\kappa = 1$, we obtain the more intuitive assumption proposed in Massart and Nédélec [2006] (see also the slightly weaker condition proposed in Kohler and Krzyżak [2007]):

MA(2) There exists $h \in]0, 1[$ such that

$$P(|2\eta(X) - 1| \leq h) = 0. \quad (8)$$

2.3 Tree classifiers, classes of tree classifiers

A tree T is a structure that can be represented as a hierarchy whose elements are called nodes. For binary trees, each node has either 0 or 2 children (called Left and Right). The initial node is called the root of the tree and a node with no child is called a leaf. The size of tree T is defined as the number of its leaves and noted $|T|$ in the following. In this paper, we define a tree $T_{c\ell}$ by two elements:

- its configuration c , i.e. the hierarchy between the nodes: for instance, in Figure 1, we know that node 6 is the Left child node of node 3, and so on,
- the ordered list ℓ of variables that appear at each node, i.e. the k^{th} variable in the list appears in node k .

A tree classifier f based on tree $T_{c\ell}$ associates

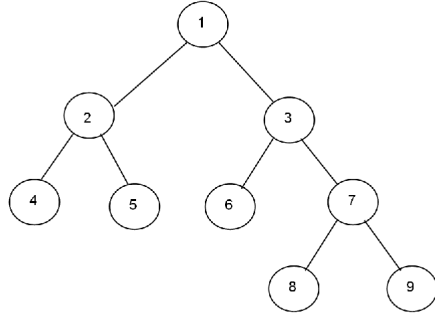


Figure 1: Tree configuration example: for each node, the parent and child nodes are known.

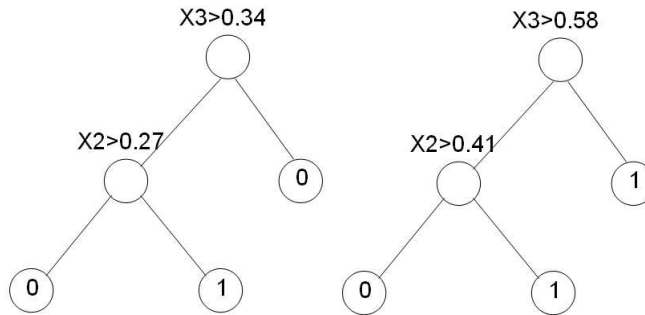


Figure 2: Two tree classifiers that belong to the same class.

- at each internal node a condition of the form " $X^{j_k} > s^k$ ", where j_k is the index of the variable associated with node k and s^k is a threshold,
- at each terminal node a label (here 0 or 1).

Therefore, an observation $x \in \mathcal{X}$ will be classified as follows: starting at the root, observation x will move from a node of f to another using the following rule: at node k , if " $x^{j_k} > s^k$ " then x moves to Right, otherwise it moves to Left. At the end of the process, x will be classified according to the label of the leaf it reaches.

To summarize, a tree classifier associated with tree T_{cl} splits \mathcal{X} into $|T_{cl}|$ regions each associated with a label, and two classifiers associated with the same tree T_{cl} differ in that the thresholds (for internal nodes) and labels (for leaves) are not the same. An example of two such tree classifiers is given in Figure 2. In the following, we will consider classes $\mathcal{C}_{cl} = \{f / f \text{ based on } T_{cl}\}$ of classifiers based on a same tree T_{cl} . Finally, we define

$$\bar{f}_{cl} \in \arg \min_{f \in \mathcal{C}_{cl}} Pf, \quad (9)$$

where Pf is defined by (2).

3 Results

3.1 Risk bounds

We first consider a single class \mathcal{C}_{cl} of tree classifiers and its associated empirical risk minimizer

$$\widehat{f}_{cl} \in \arg \min_{f \in \mathcal{C}_{cl}} P_n f,$$

where $P_n f$ is defined by (6).

Proposition 1. *Assume that margin assumption **MA(1)** is verified. For all $t_{cl} > 0$ and $\alpha > 0$, there exist positive constants K^1, K^2, K depending on α and κ such that, with probability at least $1 - e^{-t_{cl}}$,*

$$l(f^*, \widehat{f}_{cl}) \leq (1 + \alpha)l(f^*, \bar{f}_{cl}) + K^1 \left(\frac{|T_{cl}| \log(2n)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + K^2 \left(\frac{t_{cl}}{n} \right)^{\frac{\kappa}{2\kappa-1}} + K \frac{t_{cl}}{n} . \quad (10)$$

Moreover, we obtain the following upper bound

$$E \left[l(f^*, \widehat{f}_{cl}) \right] \leq (1 + \alpha)l(f^*, \bar{f}_{cl}) + K^1 \left(\frac{|T_{cl}| \log(2n)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + C n^{-\frac{\kappa}{2\kappa-1}} . \quad (11)$$

The obtained bound is in keeping with classical results already given in [Mammen and Tsybakov \[1999\]](#). In particular, if the Bayes classifier belongs to class \mathcal{C}_{cl} , the rate of convergence for the risk associated with estimator \widehat{f}_{cl} is of order $(\log(2n)/n)^{\frac{\kappa}{2\kappa-1}}$.

In practice, since no information is available about how to choose class \mathcal{C}_{cl} , one needs to consider the collection \mathcal{M} of all possible configurations and variable lists. In each class \mathcal{C}_{cl} , a candidate \widehat{f}_{cl} is chosen by empirical risk minimization, then the final classifier \tilde{f} is selected among all class candidates by minimization of a penalized criterion:

$$\begin{aligned} \widehat{cl} &= \arg \min_{c, \ell} \left(P_n \widehat{f}_{cl} + pen(c, \ell) \right) , \\ \tilde{f} &= \widehat{f}_{\widehat{cl}} . \end{aligned}$$

The following result provides insight about how the penalty should be chosen to ensure good performance for \tilde{f} .

Proposition 2. *Assume that margin assumption **MA(1)** is verified. If*

$$\tilde{f} = \underset{\{\widehat{f}_{cl}, (c, \ell) \in \mathcal{M}\}}{\operatorname{argmin}} \left(P_n \widehat{f}_{cl} + pen(c, \ell) \right), \quad (12)$$

where

$$pen(c, \ell) = C_\kappa^1 \left(\frac{|T_{cl}| \log(2n)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + C_\kappa^2 \left(\frac{|T_{cl}| \log(p)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + C_\kappa^3 \left(\frac{|T_{cl}| \log(p)}{n} \right) \quad (13)$$

with constants $C_\kappa^1, C_\kappa^2, C_\kappa^3$ depending on κ appearing in the margin condition, then there exist positive constants C'_1, C'_2 and Σ such that with probability at least $1 - 3\Sigma e^{-x}$

$$l(f^*, \tilde{f}) \leq C'_1 \inf_{c, \ell} \left\{ \inf_{f \in \mathcal{C}_{cl}} l(f^*, f) + pen(c, \ell) \right\} + C'_2 \left(\left(\frac{x}{n} \right)^{\frac{\kappa}{2\kappa-1}} + \frac{x}{n} \right) .$$

Moreover, we obtain the following upper bound:

$$\mathbb{E}[l(f^*, \tilde{f})] \leq C'_1 \inf_{(c, \ell) \in \mathcal{M}} \left\{ \inf_{f \in \mathcal{C}_{c\ell}} l(f^*, f) + \text{pen}(c, \ell) \right\} + \frac{C''_2 \times \Sigma}{n^{\frac{\kappa}{2\kappa-1}}}. \quad (14)$$

The proofs of Propositions 1 and 2 are given in Section 5.

Several comments can be made about the result of Proposition 2:

Strong margin assumption In the particular case of margin assumption **MA(2)** given by equation (8), penalty (13) becomes (taking $\kappa = 1$):

$$\begin{aligned} \text{pen}(c, \ell) &= \frac{C_h^1 \log(2n) + C_h^2 \log(p)}{n} |T_{c\ell}| \\ &= \alpha_n |T_{c\ell}|. \end{aligned}$$

This corresponds exactly to the penalty proposed in Breiman et al. [1984] for the CART algorithm (see equation (1)). A similar result was obtained in Gey and Nedelec [2005] in the regression framework, and in the binary classification context in Gey [2010], with the difference that the risk bounds were obtained conditionally on the construction of the maximal tree. Consequently, in this previous result the embedded variable selection process of the algorithm was not taken into account.

Variable selection Compared with previous results obtained for CART, equation (13) exhibits a penalty where the number of variables p explicitly appears. Moreover, the penalty term can be upper bounded by

$$\text{pen}(c, \ell) \leq C_\kappa^1 \left(\frac{|T_{c\ell}| \log(2n)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + \log(p) \left(C_\kappa^2 \left(\frac{|T_{c\ell}|}{n} \right)^{\frac{\kappa}{2\kappa-1}} + C_\kappa^3 \frac{|T_{c\ell}|}{n} \right),$$

advocating for a penalty that should be linear with respect to $\log(p)$. This linear relationship is investigated in Section 3.2.

Oracle-type inequality Vapnik's bounds for binary classification without any margin assumption give the following penalty form (see Devroye et al. [1996] for instance)

$$\text{pen}_V(c, \ell) = C_V^1 \sqrt{\frac{|T_{c\ell}| \log(n)}{n}} + C_V^2 \frac{|T_{c\ell}|}{n}.$$

This implies that, for classes associated with trees of large size, $\text{pen}(c, \ell)$ given in (13) becomes larger than $\text{pen}_V(c, \ell)$. Therefore, to obtain an oracle-type inequality, $\text{pen}(c, \ell)$ can be replaced by $\min \{ \text{pen}_V(c, \ell), \text{pen}(c, \ell) \}$.

3.2 Illustration on simulated data

3.2.1 Practical determination of \tilde{f}

The application of the strategy described in Proposition 2 necessitates finding the empirical risk minimizer in each class $\mathcal{C}_{c\ell}$, and then comparing all the candidates $\hat{f}_{c\ell}$ using the penalized criterion given by (12). From a computational point of view, the exhaustive comparison

among all classes is an NP-hard problem. Therefore we need heuristic algorithms to obtain a sequence of near-optimal penalized risk minimizers $(\widehat{f}_k)_{k \geq 1}$ such that

$$\widehat{f}_k \approx \operatorname{argmin}_{\{\widehat{f}_{c\ell}, |T_{c\ell}|=k\}} P_n \widehat{f}_{c\ell} .$$

The CART algorithm, when applied with the empirical risk as an impurity measure at each node (see [Hastie et al. \[2001\]](#)), may be understood as a forward heuristic algorithm to build the sequence of optimal tree classifiers. In particular, the subtree classifier \widehat{f}_k of size k extracted from the maximal tree can be interpreted as the (approximate) optimizer of the empirical risk over all the possible trees of size k .

This new understanding of the CART algorithm as a heuristic approach to obtain the sequence of subtree minimizers is important, because it points out that these subtree classifiers \widehat{f}_k should be penalized as if the exhaustive search were performed, *i.e.* using penalty given by (13).

In most applications, when dealing with the construction of a tree classifier, experimenters use a growing-pruning strategy where criterion (1) is used, and the unknown parameter α_n is chosen by hold-out or Q-fold cross-validation. This estimated value can be compared with its theoretical counterpart given in (13). To this end, we perform a simulation study and compare the α_n obtained by cross-validation to its theoretical form

$$\frac{C_h^1 \log(2n) + C_h^2 \log(p)}{n}$$

obtained under the strong margin assumption **MA(2)**.

3.2.2 Simulations

We consider four simulation designs:

Design 1 Variables X^1, \dots, X^p are independently generated with distribution $\mathcal{N}(0, 1)$. The label is generated as follows: If $X^1 > 0$ and $X^2 > 0$ then $Y = 1$ with probability q , otherwise $Y = 1$ with probability $1 - q$. Therefore only variables X^1 and X^2 are informative. In this design, the Bayes classifier can be represented as a tree with 3 leaves, hence it belongs to the considered collection of classes. Moreover, variables are independent, and margin assumption **MA(2)** is satisfied.

Design 2 First the labels are generated according to a Bernoulli distribution with parameter $1/2$. Then variable X^1 is generated such that $X^1|Y = 0$ and $X^1|Y = 1$ are normally distributed with means 0 and 1, respectively, and variance σ^2 . Variables X^2, \dots, X^p are independent with distribution $\mathcal{N}(0, 1)$ and are non-informative. As for design 1, the Bayes classifier can be represented as a tree and variables are independent, but it is easy to show that margin assumption **MA(2)** is not satisfied.

Design 3 Labels are simulated as in design 2. Then variables X^1 and X^2 are generated such that, for $j = 1, 2$, $X^j|Y = 0$ and $X^j|Y = 1$ are normally distributed with means 0 and 1, respectively, and variance σ^2 . The last $p - 2$ variables are independent and non-informative.

Here the Bayes classifier no longer belongs to the collection of tree classes, and margin assumption **MA(2)** is not satisfied.

Design 4 Three independent variables X^1, X^2, X^3 are generated with distribution $\mathcal{N}(0, 1)$. Each additional variable X^j is then simulated as a noisy copy of $(X^1 + X^2 + X^3)/\sqrt{3}$. The label is generated as follows: If $(X^1)^2 + (X^2)^2 + (X^3)^2 > 2.5$ then $Y = 1$, else $Y = 0$. Here, all the variables are correlated (with a strong correlation between the extra variables), the Bayes classifier cannot be represented as a tree, and margin assumption **MA(2)** is not satisfied.

For designs 1 to 3, 400 samples are generated, and 1000 for design 4. On each of them, a tree classifier is selected using the growing/pruning strategy, where parameter α_n is selected by 10-fold cross-validation. Different values of parameters n ($n = 50, 100, 200$) and noise ($q = 0.1, 0.2, 0.3$ in design 1, $\sigma^2 = 0.5, 1, 2$ in designs 2 and 3, and $\sigma^2 = 0.2$ in design 4) are used. The number of variables considered to build the classifiers grows from $p = 30$ to $p = 10^3$.

Figure 3 displays the average value (on 400 simulations) of α_n versus the log-number of variables for the different designs. Parameter α_n decreases with respect to n , and the relationship between the selected α_n and $\log p$ is linear. These behaviors are observed whatever the level of noise (not shown) and whatever the design. This confirms that variable selection is taken into account by the pruning procedure of the CART algorithm through the choice of α_n . This also suggests that the penalty function proposed in (13) is relevant regarding its dependency on $\log p$.

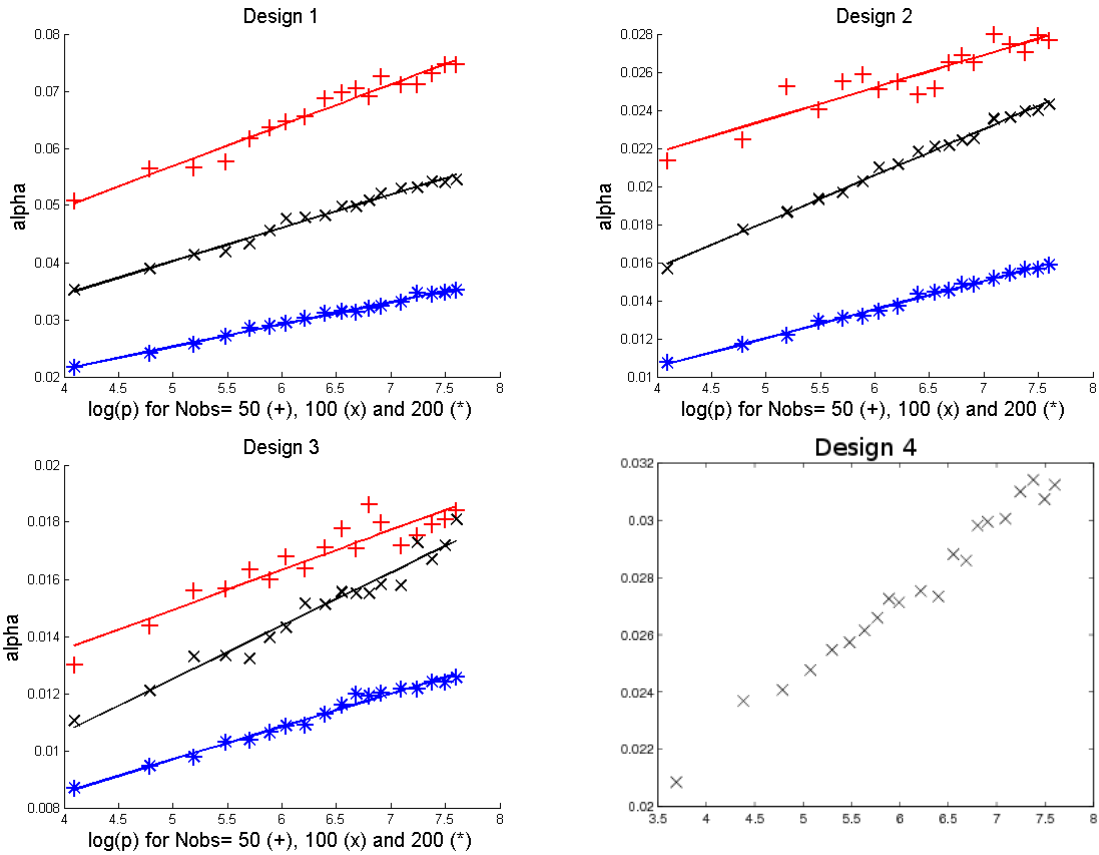


Figure 3: Average value of α_n with respect to $\log p$, for $n = 50$ (+), $n = 100$ (x) and $n = 200$ (*). Data are simulated from design 1 with $q = 0.3$ (Top Left), design 2 (Top Right), design 3 (Bottom Left) with $\sigma^2 = 2$. For design 4 (Bottom Right) the average α_n is obtained over 1000 samples, for $n = 100$.

4 Discussion

How can the risk bound presented in section 3 be related to previous results? In Gey [2010] and Nobel [2002], the collection of models includes classes $\mathcal{C}_0, \dots, \mathcal{C}_{K-1}, \mathcal{C}_K$ of tree classifiers built on the maximal tree T_K , and its subtrees $T_0 \preceq \dots \preceq T_{K-1}$. Hence the collection itself depends on the data at hand, since T_K is obtained from the training set. Thus the conditional risk bounds provided in previous articles only guarantee that the risk of the candidate is at most of the order of the risk of class \mathcal{C}_{k^*} corresponding to the best subtree T_{k^*} . While this exactly describes the process of the CART algorithm, the guarantee may be poor if the best subtree of the collection is far from the best tree among all possible trees. Conversely, the approach presented here guarantees that the risk bound for the selected tree classifier is comparable to the risk of the class corresponding to the optimal tree (among all possible trees), but this theoretical candidate may not correspond to the practical candidate identified by the algorithm used (which could be other than CART). In the two cases, the pertinence of the result relies on the quality of the algorithm itself.

The theoretical form of the penalty term (13) derived in Proposition 2 is of much practical

interest. First, it shows that sequential selection algorithms, such as stepwise or backward variable selection methods, can be easily studied in the model selection framework where the selection is supposed to be exhaustive. In the particular case of tree classification, the simulation study confirms that the penalty derived under the hypothesis of exhaustive variable selection is the one that is used in practice by the CART algorithm, that proceeds as a forward variable selection process. Second, it provides an interesting insight into the CART variable selection process. Indeed, the definition of the classes comes from the fact that a single variable may appear at different nodes, a specificity that changes the classical way of taking into account variable selection in the penalty term (see Remark in Section 5.1).

In Koltchinskii [2006a], Koltchinskii provides a synthesis of oracle inequalities in classification. In particular, the author considers margin assumptions more general than the margin assumption **MA(1)** given in Mammen and Tsybakov [1999]. The in-probability upper bounds for the loss $l(f^*, \tilde{f})$ given in Propositions 1 and 2 can be straightforwardly generalized using Koltchinskii's margin definition. This would lead to improved in-probability upper bounds for the loss $l(f^*, \tilde{f})$, similar to the one given in Theorem 6 of Koltchinskii [2006a]. However, unlike hypothesis **MA(1)** considered here, it would not permit one to obtain explicit rates of convergence for the risk. Importantly, using a more general margin assumption would provide no improvement concerning the embedded selection aspect that we investigated here. From this aspect the results obtained are tight, as illustrated by the simulation study.

5 Proofs

5.1 Preliminary results

We provide two lemmas regarding the Vapnik entropy and the cardinality of tree class collections.

We note H_{cl} the Vapnik-Chervonenkis log-entropy of class \mathcal{C}_{cl} .

Lemma 1. *For a tree class \mathcal{C}_{cl} , one has*

$$E(H_{cl}) \leq |T_{cl}| \log(2n)$$

This is obtained from lemma (2) in Gey and Nédélec [2005]. For a tree with $|T_{cl}|$ leaves, there are $|T_{cl}| - 1$ nodes for which the thresholds have to be estimated, leading to at most n ways to split the training sample. The possible number of splittings is bounded by $n^{|T_{cl}|-1}$. A given splitting shatters the sample into $|T_{cl}|$ subsamples, and each of these subsamples receive label 0 or 1. There are $2^{|T_{cl}|}$ ways to label the subsamples, hence

$$\begin{aligned} H_{cl} &< \log \left(n^{|T_{cl}|-1} \times 2^{|T_{cl}|} \right) \\ &< |T_{cl}| \log(2n) . \end{aligned}$$

Taking the expectation leads to the result.

Lemma 2. *The number of classes of trees of size k is*

$$p^{k-1} N_{(k)}, \quad \text{with} \quad N_{(k)} = \frac{1}{k} \binom{2k-2}{k-1} .$$

First note that counting the number of classes amounts to counting the number of trees. A tree $T_{c\ell}$ is defined by a configuration c combined with a variable list ℓ . The total number of tree configurations of size k is given by the Catalan number $N_{(k)}$. The total number of lists of $k - 1$ variables is p^{k-1} , because at each node we have to choose between the p available variables. Combined with the total number of tree configurations, this leads to the proposed lemma.

Remark In contrast with the classical variable selection framework, in trees the variable list is ordered (the first variable of the list is associated with the first node) and a variable may be associated with several nodes. Therefore the classical $\binom{p}{k-1}$ term that appears in penalties in [Birgé and Massart \[2001\]](#) or [Mary-Huard et al. \[2007\]](#) (i.e. the number of samplings without replacements and unordered sample) is replaced with p^{k-1} (i.e. the number of sampling with replacements and ordered sample).

5.2 Proof of Proposition 1

A classical way to bound $l(f^*, \widehat{f}_{c\ell})$ is to use the following decomposition:

$$l(f^*, \widehat{f}_{c\ell}) = l(f^*, \bar{f}_{c\ell}) + P\widehat{f}_{c\ell} - P\bar{f}_{c\ell},$$

and then to upper bound the variance term $P\widehat{f}_{c\ell} - P\bar{f}_{c\ell}$. This last step can be done using Theorem 2 from [Koltchinskii \[2006a\]](#), which can be restated for our purpose as follows:

Theorem 5.2.1 (Koltchinskii, 2006). *If there exists a nondecreasing strictly concave function $\psi_{c\ell} : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ such that with probability at least $1 - e^{-t_{c\ell}}$*

$$\sup_{f, g \in \mathcal{C}_{c\ell}(\delta)} |(P_n - P)(f - g)| \leq \psi_{c\ell}(\delta) \quad ,$$

and if $\psi_{c\ell}^\sharp$ is defined as

$$\psi_{c\ell}^\sharp(\varepsilon) = \inf\{\delta > 0 \text{ s.t. } \sup_{\sigma \geq \delta} \frac{\psi(\sigma)}{\sigma} \leq \varepsilon\} \quad ,$$

then for all $\delta \geq \psi_{c\ell}^\sharp(1/q)$

$$P \left[P\widehat{f}_{c\ell} - P\bar{f}_{c\ell} > \delta \right] \leq e^{-t_{c\ell}} \quad .$$

In order to use Theorem 5.2.1, we need to provide an explicit expression for $\psi_{c\ell}$. To proceed, we start from the following probabilistic upper bound given in [Koltchinskii \[2006a\]](#) and derived from Talagrand's inequality for bounded processes (see [Bousquet \[2002\]](#) for more details):

$$\sup_{f, g \in \mathcal{C}_{c\ell}(\delta)} |(P_n - P)(f - g)| \leq 2 \left(\mathbb{E} \left[\sup_{f, g \in \mathcal{C}_{c\ell}(\delta)} |(P_n - P)(f - g)| \right] + D(\mathcal{C}_{c\ell}(\delta)) \sqrt{\frac{t_{c\ell}}{n} + \frac{t_{c\ell}}{n}} \right) \quad (15)$$

with probability larger than $1 - e^{-t_{c\ell}}$, where

$$\mathcal{C}_{c\ell}(\delta) = \{f \in \mathcal{C}_{c\ell} \text{ s.t. } Pf - P\bar{f}_{c\ell} \leq \delta\}$$

and

$$\begin{aligned} D(\mathcal{C}_{cl}(\delta)) &= \sup_{f,g \in \mathcal{C}_{cl}(\delta)} \sqrt{\mathbb{E}((f-g)^2)} \\ &= \sup_{f,g \in \mathcal{C}_{cl}(\delta)} d(f,g) \end{aligned}$$

This last term can be upper-bounded in expression (15) using the margin assumption **MA(1)** described by (7):

$$d^2(f, f^*) \leq C_\kappa l(f^*, f)^{\frac{1}{\kappa}}$$

where $C_\kappa = (\kappa - 1)^{\frac{1}{\kappa}} C^{\frac{\kappa-1}{\kappa}} \frac{\kappa}{\kappa-1}$. Hence

$$\begin{aligned} d(f, g) &\leq 2\sqrt{C_\kappa} \left(l(f^*, \bar{f}_{cl})^{\frac{1}{2\kappa}} + \delta^{\frac{1}{2\kappa}} \right) \\ \Rightarrow D(\mathcal{C}_{cl}(\delta)) &\leq 2\sqrt{C_\kappa} \left(l(f^*, \bar{f}_{cl})^{\frac{1}{2\kappa}} + \delta^{\frac{1}{2\kappa}} \right) = D. \end{aligned} \quad (16)$$

Now because

$$\mathbb{E} \left[\sup_{f,g \in \mathcal{C}_{cl}(\delta)} |(P_n - P)(f-g)| \right] \leq \mathbb{E} \left[\sup_{d(f,g) \leq D} |(P_n - P)(f-g)| \right]$$

we can use the result of [Massart \[2000\]](#) (p295) to obtain

$$\mathbb{E} \left[\sup_{f,g \in \mathcal{C}_{cl}(\delta)} |(P_n - P)(f-g)| \right] \leq 24D \sqrt{\frac{E[H_{cl}]}{n}}, \quad (17)$$

where H_{cl} is the Vapnik-Chervonenkis log-entropy of \mathcal{C}_{cl} . Combining (16) and (17), then using lemma 5 of [Tsybakov and van de Geer \[2005\]](#), we obtain for all $\alpha \in]0, 1[$

$$\begin{aligned} \sup_{f,g \in \mathcal{C}_{cl}(\delta)} |(P_n - P)(f-g)| &\leq 2 \left[2\sqrt{C_\kappa} \left(24\sqrt{\frac{E[H_{cl}]}{n}} + \sqrt{\frac{t_{cl}}{n}} \right) \left(l(f^*, \bar{f}_{cl})^{\frac{1}{2\kappa}} + \delta^{\frac{1}{2\kappa}} \right) + \frac{t_{cl}}{n} \right] \\ &\leq 4\sqrt{C_\kappa} \left(24\sqrt{\frac{E[H_{cl}]}{n}} + \sqrt{\frac{t_{cl}}{n}} \right) \delta^{\frac{1}{2\kappa}} \\ &\quad + 2\frac{t_{cl}}{n} + \alpha l(f^*, \bar{f}_{cl}) + \beta_{\kappa,\alpha} \left(\frac{E[H_{cl}]}{n} \right)^{\frac{\kappa}{2\kappa-1}} + \frac{\beta_{\kappa,\alpha}}{24} \left(\frac{t_{cl}}{n} \right)^{\frac{\kappa}{2\kappa-1}}. \end{aligned}$$

In the present framework, we then have

$$\begin{aligned} \psi_{cl}(\delta) &= 4\sqrt{C_\kappa} \left(24\sqrt{\frac{E[H_{cl}]}{n}} + \sqrt{\frac{t_{cl}}{n}} \right) \delta^{\frac{1}{2\kappa}} + 2\frac{t_{cl}}{n} + \alpha l(f^*, \bar{f}_{cl}) + \beta_{\kappa,\alpha} \left(\frac{E[H_{cl}]}{n} \right)^{\frac{\kappa}{2\kappa-1}} + \frac{\beta_{\kappa,\alpha}}{24} \left(\frac{t_{cl}}{n} \right)^{\frac{\kappa}{2\kappa-1}} \\ &= \psi_1(\delta) + \psi_2(\delta) + K \end{aligned}$$

where

$$\begin{aligned} \psi_1(\delta) &= 96\sqrt{C_\kappa} \sqrt{\frac{E[H_{cl}]}{n}} \delta^{\frac{1}{2\kappa}} \\ \psi_2(\delta) &= 4\sqrt{C_\kappa} \sqrt{\frac{t_{cl}}{n}} \delta^{\frac{1}{2\kappa}} \\ \text{and } K &= 2\frac{t_{cl}}{n} + \alpha l(f^*, \bar{f}_{cl}) + \beta_{\kappa,\alpha} \left(\frac{E[H_{cl}]}{n} \right)^{\frac{\kappa}{2\kappa-1}} + \frac{\beta_{\kappa,\alpha}}{24} \left(\frac{t_{cl}}{n} \right)^{\frac{\kappa}{2\kappa-1}} \end{aligned}$$

Moreover, $\psi_{cl}^\sharp(\varepsilon) \leq \psi_1^\sharp(\varepsilon/3) + \psi_1^\sharp(\varepsilon/3) + \frac{3K}{\varepsilon}$, and ψ_1^\sharp and ψ_2^\sharp can be determined using the following characterization (available for all strictly concave functions ψ):

$$\forall \varepsilon > 0, \psi\left(\psi^\sharp(\varepsilon)\right) = \psi^\sharp(\varepsilon)\varepsilon \ .$$

Solving this last equation for the particular form of functions ψ_1 and ψ_2 , we obtain

$$\begin{aligned} \psi_{cl}^\sharp(\varepsilon) \leq & \left(\frac{288\sqrt{C_\kappa}\sqrt{E[H_{cl}]}}{\varepsilon\sqrt{n}} \right)^{\frac{2\kappa}{2\kappa-1}} + \left(\frac{12\sqrt{C_\kappa}\sqrt{t_{cl}}}{\varepsilon\sqrt{n}} \right)^{\frac{2\kappa}{2\kappa-1}} \\ & + \left(2\frac{t_{cl}}{n} + \alpha l(f^*, \bar{f}_{cl}) + \beta_{\kappa,\alpha} \left(\frac{E[H_{cl}]}{n} \right)^{\frac{\kappa}{2\kappa-1}} + \frac{\beta_{\kappa,\alpha}}{24} \left(\frac{t_{cl}}{n} \right)^{\frac{\kappa}{2\kappa-1}} \right) \frac{3}{\varepsilon} \end{aligned}$$

Taking $\varepsilon = 1/q$ one has with probability larger than $1 - e^{-t_{cl}}$

$$\begin{aligned} P\widehat{f}_{cl} - P\bar{f}_{cl} \leq & \left((q288\sqrt{C_\kappa})^{\frac{2\kappa}{2\kappa-1}} + 3q\beta_{\kappa,\alpha} \right) \left(\frac{E[H_{cl}]}{n} \right)^{\frac{\kappa}{2\kappa-1}} + \left((q12\sqrt{C_\kappa})^{\frac{2\kappa}{2\kappa-1}} + \frac{3q\beta_{\kappa,\alpha}}{24} \right) \left(\frac{t_{cl}}{n} \right)^{\frac{\kappa}{2\kappa-1}} \\ & + 6q\frac{t_{cl}}{n} + 3q\alpha l(f^*, \bar{f}_{cl}) \ . \end{aligned}$$

Using Lemma 1 and rescaling α properly, this leads to

$$l(f^*, \widehat{f}_{cl}) \leq (1 + \alpha)l(f^*, \bar{f}_{cl}) + K_{\alpha,\kappa,q}^1 \left(\frac{|T_{cl}|\log(2n)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + K_{\alpha,\kappa,q}^2 \left(\frac{t_{cl}}{n} \right)^{\frac{\kappa}{2\kappa-1}} + K_q \frac{t_{cl}}{n} \ . \quad (18)$$

Renaming $K_{\alpha,\kappa,q}^1 = K^1$, $K_{\alpha,\kappa,q}^2 = K^2$ and $K_q = K$ leads to the first expression in Proposition 1. The risk bound follows by integration.

5.3 Proof of Proposition 2

We first choose the weights $t_{cl} = x_{cl} + x$ associated with classes \mathcal{C}_{cl} such that x_{cl} and x are positive and

$$\sum_{c,l} e^{-x_{cl}} = \Sigma < +\infty \ .$$

The exact form of the weights will be chosen later. Furthermore, we will use lemma 4 of Koltchinskii [2006a], reformulated here for our purpose:

Lemma 5.3.1 (Koltchinskii, 2006). *Consider a class \mathcal{C}_{cl} . For all $t_{cl} > 0$ and $\alpha \in]0, 2/5[$, with probability at least $1 - 2e^{-t_{cl}}$, one has*

$$P_n \bar{f}_{cl} - P_n f^* \leq (1 + \alpha)(P \bar{f}_{cl} - P f^*) + K_\alpha \left(\frac{t_{cl}}{n} \right)^{\frac{\kappa}{2\kappa-1}} + \frac{t_{cl}}{n} \quad (19)$$

and

$$P \bar{f}_{cl} - P f^* \leq \left(1 - \frac{5}{2}\alpha \right)^{-1} \left(P_n \widehat{f}_{cl} - P_n f^* + \frac{3}{2}K^1 \left(\frac{|T_{cl}|\log(2n)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 3K^2 \left(\frac{t_{cl}}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 3K \frac{t_{cl}}{n} \right) \quad (20)$$

with the same notations as above.

We start the proof from the result obtained in Proposition 1. Combining equation (10) of Proposition 1 and a classical union bound argument, one has with probability larger than $1 - \Sigma e^{-x}$

$$l(f^*, \tilde{f}) \leq (1 + \alpha)l(f^*, \bar{f}_{\widehat{c\ell}}) + K^1 \left(\frac{|T_{\widehat{c\ell}}| \log(2n)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + K^2 \left(\frac{x_{\widehat{c\ell}} + x}{n} \right)^{\frac{\kappa}{2\kappa-1}} + K \frac{x_{\widehat{c\ell}} + x}{n} ,$$

where $\alpha \in]0, 2/5[$. We now use equation (20) from Lemma 5.3.1 to obtain with probability larger than $1 - 3\Sigma e^{-x}$

$$\begin{aligned} l(f^*, \tilde{f}) &\leq \frac{(1 + \alpha)}{1 - \frac{5\alpha}{2}} \left(\mathbb{P}_n \widehat{f}_{\widehat{c\ell}} - \mathbb{P}_n f^* + \frac{5K^1}{2} \left(\frac{|T_{\widehat{c\ell}}| \log(2n)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 4K^2 \left(\frac{x_{\widehat{c\ell}} + x}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 4K \frac{x_{\widehat{c\ell}} + x}{n} \right) \\ &\leq \frac{(1 + \alpha)}{1 - \frac{5\alpha}{2}} \left(\mathbb{P}_n \widehat{f}_{\widehat{c\ell}} - \mathbb{P}_n f^* + \frac{5K^1}{2} \left(\frac{|T_{\widehat{c\ell}}| \log(2n)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 4K^2 \left(\frac{x_{\widehat{c\ell}}}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 4K \frac{x_{\widehat{c\ell}}}{n} \right) \\ &\quad + \frac{(1 + \alpha)}{1 - \frac{5\alpha}{2}} \left(4K^2 \left(\frac{x}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 4K \frac{x}{n} \right) \end{aligned}$$

In the context of variable selection, one has to choose the weights such that

$$\sum_{c,l} e^{-x_{cl}} < +\infty \Rightarrow \sum_k \sum_{\mathcal{C}_{cl} \text{ s.t. } |T_{cl}|=k} e^{-x_{cl}} < +\infty .$$

Giving equal weights x_k to classes of same complexity k (i.e. classes \mathcal{C}_{cl} and $\mathcal{C}_{c'l'}$ such that $|T_{cl}| = |T_{c'l'}| = k$), one obtains from Lemma 2:

$$\begin{aligned} \sum_k \sum_{\mathcal{C}_{cl} \text{ s.t. } |T_{cl}|=k} e^{-x_{cl}} &= \sum_k p^{k-1} \frac{1}{k} \binom{2k-2}{k-1} e^{-x_k} \\ &\leq \sum_k \frac{(4p)^k}{k} e^{-x_k} . \end{aligned}$$

The choice $x_{cl} = x_{|T_{cl}|} = \lambda |T_{cl}| \log(p)$ with $\lambda > 3$ ensures that the sum is finite. Hence,

$$\begin{aligned} l(f^*, \tilde{f}) &\leq \frac{(1 + \alpha)}{1 - \frac{5\alpha}{2}} \left(\mathbb{P}_n \widehat{f}_{\widehat{c\ell}} - \mathbb{P}_n f^* + \frac{5K^1}{2} \left(\frac{|T_{\widehat{c\ell}}| \log(2n)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 4K^2 \left(\frac{\lambda |T_{\widehat{c\ell}}| \log(p)}{n} \right)^{\frac{\kappa}{2\kappa-1}} \right. \\ &\quad \left. + 4K \frac{\lambda |T_{\widehat{c\ell}}| \log(p)}{n} \right) + \frac{(1 + \alpha)}{1 - \frac{5\alpha}{2}} \left(4K^2 \left(\frac{x}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 4K \frac{x}{n} \right) \\ &\leq \frac{(1 + \alpha)}{1 - \frac{5\alpha}{2}} \left(\mathbb{P}_n \widehat{f}_{\widehat{c\ell}} - \mathbb{P}_n f^* + C_\kappa^1 \left(\frac{|T_{\widehat{c\ell}}| \log(2n)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + C_\kappa^2 \left(\frac{|T_{\widehat{c\ell}}| \log(p)}{n} \right)^{\frac{\kappa}{2\kappa-1}} + C_\kappa^3 \left(\frac{|T_{\widehat{c\ell}}| \log(p)}{n} \right) \right) \\ &\quad + \frac{(1 + \alpha)}{1 - \frac{5\alpha}{2}} \left(4K^2 \left(\frac{x}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 4K \frac{x}{n} \right) , \end{aligned}$$

for a proper choice of constants C_κ^1 , C_κ^2 , and C_κ^3 . This leads to

$$l(f^*, \tilde{f}) \leq \frac{(1 + \alpha)}{1 - \frac{5\alpha}{2}} \inf_{c,l} \left(\mathbb{P}_n \widehat{f}_{cl} - \mathbb{P}_n f^* + pen(c, \ell) \right) + \frac{(1 + \alpha)}{1 - \frac{5\alpha}{2}} \left(4K^2 \left(\frac{x}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 4K \frac{x}{n} \right) .$$

Since $P_n \widehat{f}_{cl} - P_n f^* \leq P_n \bar{f}_{cl} - P_n f^*$ (by definition of \widehat{f}_{cl}), this last expression can be upper bounded (with probability larger than $1 - 3\Sigma e^{-x}$) thanks to equation (19) of Lemma 5.3.1:

$$\begin{aligned}
l(f^*, \tilde{f}) &\leq \frac{(1+\alpha)^2}{1-\frac{5\alpha}{2}} \inf_{c,l} \left(P \bar{f}_{cl} - P f^* + K_\alpha \left(\frac{x_{cl}}{n} \right)^{\frac{\kappa}{2\kappa-1}} + \left(\frac{x_{cl}}{n} \right) + K_\alpha \left(\frac{x}{n} \right)^{\frac{\kappa}{2\kappa-1}} + \left(\frac{x}{n} \right) + pen(c, \ell) \right) \\
&\quad + \frac{(1+\alpha)}{1-\frac{5\alpha}{2}} \left(4K^2 \left(\frac{x}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 4K \frac{x}{n} \right) \\
&\leq \frac{2(1+\alpha)^2}{1-\frac{5\alpha}{2}} \inf_{c,l} (P \bar{f}_{cl} - P f^* + pen(c, \ell)) + \frac{2(1+\alpha)^2}{1-\frac{5\alpha}{2}} \left(4K^2 \left(\frac{x}{n} \right)^{\frac{\kappa}{2\kappa-1}} + 4K \frac{x}{n} \right) \\
&\leq C'_1 \inf_{c,l} (P \bar{f}_{cl} - P f^* + pen(c, \ell)) + C'_2 \left(\left(\frac{x}{n} \right)^{\frac{\kappa}{2\kappa-1}} + \frac{x}{n} \right).
\end{aligned}$$

The last inequality corresponds to the first equation of Proposition 2. The risk bound follows by integration.

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