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Sylvain Arlot

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# Minimal penalties and the slope heuristics: a survey

**Titre:** Pénalités minimales et heuristique de pente

Sylvain Arlot<sup>1</sup>

**Abstract:** Birgé and Massart proposed in 2001 the slope heuristics as a way to choose optimally from data an unknown multiplicative constant in front of a penalty. It is built upon the notion of minimal penalty, and it has been generalized since to some “minimal-penalty algorithms”. This article reviews the theoretical results obtained for such algorithms, with a self-contained proof in the simplest framework, precise proof ideas for further generalizations, and a few new results. Explicit connections are made with residual-variance estimators —with an original contribution on this topic, showing that for this task the slope heuristics performs almost as well as a residual-based estimator with the best model choice— and some classical algorithms such as L-curve or elbow heuristics, Mallows’  $C_p$ , and Akaike’s FPE. Practical issues are also addressed, including two new practical definitions of minimal-penalty algorithms that are compared on synthetic data to previously-proposed definitions. Finally, several conjectures and open problems are suggested as future research directions.

**Résumé :** Birgé et Massart ont proposé en 2001 l’heuristique de pente, pour déterminer à l’aide des données une constante multiplicative optimale devant une pénalité en sélection de modèles. Cette heuristique s’appuie sur la notion de pénalité minimale, et elle a depuis été généralisée en “algorithmes à base de pénalités minimales”. Cet article passe en revue les résultats théoriques obtenus sur ces algorithmes, avec une preuve complète dans le cadre le plus simple, des idées de preuves précises pour généraliser ce résultat au-delà des cadres déjà étudiés, et quelques résultats nouveaux. Des liens sont faits avec les méthodes d’estimation de la variance résiduelle (avec une contribution originale sur ce thème, qui démontre que l’heuristique de pente produit un estimateur de la variance quasiment aussi bon qu’un estimateur fondé sur les résidus d’un modèle oracle) ainsi qu’avec plusieurs algorithmes classiques tels que les heuristiques de coude (ou de courbe en L),  $C_p$  de Mallows et FPE d’Akaike. Les questions de mise en œuvre pratique sont également étudiées, avec notamment la proposition de deux nouvelles définitions pratiques pour des algorithmes à base de pénalités minimales et leur comparaison aux définitions précédentes sur des données simulées. Enfin, des conjectures et problèmes ouverts sont proposés comme pistes de recherche pour l’avenir.

**Keywords:** model selection, estimator selection, penalization, slope heuristics, minimal penalty, residual-variance estimation, L-curve heuristics, elbow heuristics, scree test, overpenalization

**Mots-clés :** sélection de modèles, sélection d’estimateurs, pénalisation, heuristique de pente, pénalité minimale, estimation de la variance résiduelle, heuristique de courbe en L, heuristique de coude, test scree, surpénalisation

**AMS 2000 subject classifications:** 62-02, 62G05, 62J05

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## 1. Introduction

Model selection attracts much attention in statistics since more than forty years (Akaike, 1973; Mallows, 1973; Burnham and Anderson, 2002; Massart, 2007). A related and crucial question for machine learning is the data-driven choice of hyperparameters of learning algorithms. Both are particular instances of the estimator-selection problem: given a family of estimators, how to choose from data one among them whose risk is as small as possible?

One of the main strategies proposed for estimator (or model) selection is penalization, that is, choosing the estimator minimizing the sum of its empirical risk—how well it fits the data—and some penalty term—whose role is to avoid overfitting. Optimal penalties often depend on at least

one parameter whose data-driven choice is challenging. In the early 2000s, [Birgé and Massart \(2001b, 2007\)](#) pointed out two key facts leading to a novel approach for an optimal data-driven choice of multiplicative constants in front of penalties. Birgé and Massart were considering a rather theoretical question: what is the *minimal* amount of penalization needed for avoiding a strong overfitting? For least-squares estimators in regression, they noticed that (i) the minimal penalty is equal to half the optimal penalty, and (ii) the minimal penalty is observable. These two facts are called “the slope heuristics”<sup>2</sup> and lead to an algorithm for choosing multiplicative constants in front of penalties.

These ideas and the corresponding algorithm have been generalized since to several frameworks (see Section 3–4 and 8), with numerous applications in various fields such as biology ([Reynaud-Bouret and Schbath, 2010](#); [Akakpo, 2011](#); [Bontemps and Toussile, 2013](#); [Rau et al., 2015](#); [Devijver et al., 2017](#); [Devijver and Gallopin, 2018](#)), energy ([Michel, 2008](#); [Devijver et al., 2019](#)), or text analysis ([Derman and Le Pennec, 2017](#)); Section 8.3 provides more examples of applications.

In particular, for linear estimators in regression, the original slope heuristics does not work directly and can be modified successfully into a more general “minimal-penalty algorithm” ([Arlot and Bach, 2009, 2011](#)) detailed in Section 3.

For least-squares regression with projection or linear estimators, the slope heuristics also provides a residual-variance estimator with nice properties (Section 6.1). In the general setting, the slope heuristics can also be seen as a way to give proper mathematical grounds to “L-curve” or “elbow-heuristics” algorithms that are used for choosing regularization parameters in ill-posed problems ([Hansen and O’Leary, 1993](#)), as explained in Sections 6.4–6.5.

**Goals** The goals of this survey are the following:

1. to review recent theoretical results about the slope heuristics, and more generally about all minimal-penalty algorithms (Sections 2–4);
2. to help identifying how —and under which assumptions— such results could be generalized to other settings, possibly with new algorithms, by giving a precise account of existing proofs (Sections 2.7, 4.1, and 5), and by identifying several conjectures and open problems suggested by experimental results (Section 8);
3. to make connections between minimal penalties and other classical procedures for residual-variance estimation and for model or estimator selection (Section 6).

Practical issues are only briefly mentioned in Section 7, since more details can be found on these in the survey by [Baudry et al. \(2012\)](#).

There is currently no final answer to the question of generalizing minimal-penalty algorithms as much as possible, but we hope that this survey will motivate further theoretical and empirical work in this direction, which could have a great practical impact in statistics, machine learning, and data science in general.

<sup>2</sup> In “the slope heuristics”, the word “heuristics” is an *uncountable* noun, following the Oxford Advanced Learner’s Dictionary. One could also write “the slope heuristic”, according to some other English dictionaries in which “heuristic” appears as a noun. We use the former spelling throughout this article, but some other articles make use of the latter spelling (without the final s).

**Contributions** Let us finally point out some original results appearing in this article. In the framework of least-squares fixed-design regression with projection estimators and Gaussian noise, Theorem 1 validates the slope heuristics in a stronger sense compared to previous results (Birgé and Massart, 2007); it is inspired by Arlot and Bach (2011) but makes weaker assumptions. Its extension to sub-Gaussian noise (Remark 1 in Section 2.5) is original. As a corollary, Proposition 3 in Section 6.1 is the first precise statement on a slope-heuristics-based residual-variance estimator—more precise than the result that can be derived from Arlot and Bach (2011)—, showing that it is minimax optimal (up to  $\log(n)$  factors) under mild assumptions. Proposition 3 provides non-asymptotic bounds (in expectation and with high probability) on this residual-variance estimator, that can be seen as some kind of oracle inequality for residual-variance estimation, which is interesting independently from the slope heuristics.

In the general framework, Propositions 1–2 in Section 5.2 propose two general approaches for justifying minimal-penalty algorithms. These approaches were previously proposed in specific settings (Lerasle and Takahashi, 2016; Garivier and Lerasle, 2011), but their generalization to the setting of Section 3.1 is new. For instance, the application of Proposition 1 to general minimum-contrast estimators with a bounded contrast is new, to the best of our knowledge.

On the practical side, as a complement to the survey by Baudry et al. (2012), Section 7 shows original numerical experiments on synthetic data, assessing the performance of the slope heuristics in the least-squares regression framework, for both residual-variance estimation and model selection. Two new practical definitions of the slope heuristics (called ‘median’ and ‘consensus’) are proposed and compared to the classical ones. An efficient implementation of one previously-proposed definition is also provided and proved (Algorithm 8 and Proposition 6 in Appendix B.2).

## 2. The slope heuristics

This section presents the original “slope heuristics” (Birgé and Massart, 2001b, 2007) in the framework of fixed-design regression, with the least-squares risk and projection estimators. By focusing on this framework, we get most of the flavor of the slope heuristics while keeping the exposition simple.

### 2.1. Framework

The framework considered in Section 2 is the following. We observe

$$Y = F + \varepsilon \in \mathbb{R}^n \tag{1}$$

where  $\varepsilon_1, \dots, \varepsilon_n$  are independent and identically distributed with mean 0 and variance  $\sigma^2$ , and  $F \in \mathbb{R}^n$  is some (deterministic) signal of interest. For instance,  $F$  can be equal to  $(f(x_i))_{1 \leq i \leq n}$  for some deterministic design points  $x_1, \dots, x_n \in \mathcal{X}$  and  $f$  some unknown measurable function  $\mathcal{X} \mapsto \mathbb{R}$ , with no assumption on the set  $\mathcal{X}$ .

The goal is to reconstruct  $F$  from  $Y$ , that is, to find some  $t \in \mathbb{R}^n$  such that its quadratic risk

$$\frac{1}{n} \|t - F\|^2$$

is small, where for every  $u \in \mathbb{R}^n$ ,  $\|u\|^2 = \sum_{i=1}^n u_i^2$ . To this end, for every linear subspace  $S$  of  $\mathbb{R}^n$ , the *projection estimator* or *least-squares estimator* on  $S$  is defined as

$$\widehat{F}_S \in \operatorname{argmin}_{t \in S} \left\{ \frac{1}{n} \|t - Y\|^2 \right\}$$

where  $n^{-1} \|t - Y\|^2$  is called the empirical risk of  $t$ . Since  $S$  is a linear subspace,  $\widehat{F}_S$  exists and is unique:  $\widehat{F}_S = \Pi_S Y$  where  $\Pi_S : \mathbb{R}^n \rightarrow \mathbb{R}^n$  denotes the orthogonal projection onto  $S$ . In the following, any linear subspace  $S$  of  $\mathbb{R}^n$  is called a *model*.

Let  $(S_m)_{m \in \mathcal{M}}$  be some collection of models, and for every  $m \in \mathcal{M}$ , let

$$\widehat{F}_m = \widehat{F}_{S_m} = \Pi_{S_m} Y \quad \text{and} \quad \Pi_m = \Pi_{S_m}.$$

In this survey, we assume that the goal of model selection is to choose from data some  $\widehat{m} \in \mathcal{M}$  such that the quadratic risk of  $\widehat{F}_{\widehat{m}}$  is minimal. The best choice would be the *oracle*:

$$m^* \in \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \frac{1}{n} \|\widehat{F}_m - F\|^2 \right\},$$

which cannot be used since it depends on the unknown signal  $F$ . Therefore, the goal is to define a data-driven  $\widehat{m}$  satisfying an *oracle inequality*

$$\frac{1}{n} \|\widehat{F}_{\widehat{m}} - F\|^2 \leq K_n \inf_{m \in \mathcal{M}} \left\{ \frac{1}{n} \|\widehat{F}_m - F\|^2 \right\} + R_n \quad (2)$$

with large probability, where the leading constant  $K_n$  should be close to 1 —at least for large  $n$ — and the remainder term  $R_n$  should be small compared to the oracle risk  $\inf_{m \in \mathcal{M}} \{n^{-1} \|\widehat{F}_m - F\|^2\}$ .

## 2.2. Optimal penalty

Many classical selection methods are built upon the “unbiased risk estimation” heuristics: If  $\widehat{m}$  minimizes a criterion  $\operatorname{crit}(m)$  such that

$$\forall m \in \mathcal{M}, \quad \mathbb{E}[\operatorname{crit}(m)] \approx \mathbb{E} \left[ \frac{1}{n} \|\widehat{F}_m - F\|^2 \right],$$

then  $\widehat{m}$  satisfies with large probability an oracle inequality such as Eq. (2) with an optimal constant  $K_n = 1 + o(1)$ . This can be proved by showing a concentration inequality for  $\|\Pi_m \varepsilon\|^2$  and  $\langle \varepsilon, (I_n - \Pi_m)F \rangle$  around their expectations for all  $m \in \mathcal{M}$ , where  $I_n$  denotes the identity matrix of  $\mathbb{R}^n$ , see Section 2.7. For instance, cross-validation (Allen, 1974; Stone, 1974) and generalized cross-validation (GCV; Craven and Wahba, 1978) are built upon this heuristics.

One way of implementing this heuristics is penalization, which consists of minimizing the sum of the empirical risk and a penalty term, that is, using a criterion of the form:

$$\operatorname{crit}(m) = \frac{1}{n} \|\widehat{F}_m - Y\|^2 + \operatorname{pen}(m). \quad (3)$$

The unbiased risk estimation heuristics, also called Mallows' heuristics, then leads to the *optimal (deterministic) penalty*

$$\text{pen}_{\text{opt},0}(m) := \mathbb{E} \left[ \frac{1}{n} \|\widehat{F}_m - F\|^2 \right] - \mathbb{E} \left[ \frac{1}{n} \|\widehat{F}_m - Y\|^2 \right]. \quad (4)$$

When  $\widehat{F}_m = \Pi_m Y$ , we have

$$\|\widehat{F}_m - F\|^2 = \|(I_n - \Pi_m)F\|^2 + \|\Pi_m \varepsilon\|^2 \quad (5)$$

$$\text{and} \quad \|\widehat{F}_m - Y\|^2 = \|\widehat{F}_m - F\|^2 + \|\varepsilon\|^2 - 2\langle \varepsilon, \Pi_m \varepsilon \rangle + 2\langle \varepsilon, (I_n - \Pi_m)F \rangle, \quad (6)$$

where  $\forall t, u \in \mathbb{R}^n$ ,  $\langle t, u \rangle = \sum_{i=1}^n t_i u_i$ . Since the  $\varepsilon_i$  are independent, centered, with variance  $\sigma^2$ , Eq. (5) and Eq. (6) imply that

$$\mathbb{E} \left[ \frac{1}{n} \|\widehat{F}_m - F\|^2 \right] = \frac{1}{n} \|(I_n - \Pi_m)F\|^2 + \frac{\sigma^2 D_m}{n}, \quad (7)$$

$$\mathbb{E} \left[ \frac{1}{n} \|\widehat{F}_m - Y\|^2 \right] = \frac{1}{n} \|(I_n - \Pi_m)F\|^2 + \frac{\sigma^2 (n - D_m)}{n}, \quad (8)$$

$$\text{and} \quad \text{pen}_{\text{opt},0}(m) + \sigma^2 = \frac{2\sigma^2 D_m}{n} =: \text{pen}_{\text{opt}}(m), \quad (9)$$

where  $D_m := \dim(S_m)$ . Note that the optimal penalties (9) and (4) differ by an additive constant  $\sigma^2$ , which does not change the argmin of the penalized criterion (3); this choice simplifies formulas involving  $\text{pen}_{\text{opt}}$ .

Eq. (7) is classically known as a *bias-variance decomposition of the risk*: the first term — called *approximation error* or bias— decreases when  $S_m$  gets larger, while the second term — called *estimation error* or variance— increases when  $S_m$  gets larger, see Figure 1 left. Eq. (8) shows that the expectation of the empirical risk decreases when  $S_m$  gets larger, as expected since  $\widehat{F}_m$  is defined as a minimizer of the empirical risk, see Figure 1 left.

The expression of the optimal penalty in Eq. (9) leads to Mallows'  $C_p$  (Mallows, 1973), where  $\sigma^2$  is replaced by some estimator  $\widehat{\sigma}^2$ . Several approaches exist for estimating  $\sigma^2$ , see Section 6.1. The slope heuristics provides a data-driven estimation of the unknown constant  $\sigma^2$  in front of the penalty shape  $D_m/n$  thanks to the notion of minimal penalty.

### 2.3. Minimal penalty and the slope heuristics

Eq. (9) shows that the shape  $\text{pen}_1(m) = D_m/n$  of the optimal penalty is known, even when  $\sigma^2$  is unknown. A natural question is to determine the minimal value of the constant that should be put in front of  $\text{pen}_1(m)$ . More precisely, if for every  $C \geq 0$

$$\widehat{m}(C) \in \underset{m \in \mathcal{M}}{\text{argmin}} \left\{ \frac{1}{n} \|\widehat{F}_m - Y\|^2 + C \frac{D_m}{n} \right\}, \quad (10)$$

what is the minimal value of  $C$  such that  $\widehat{m}(C)$  stays a “reasonable” choice, that is, avoids strong overfitting, or equivalently, satisfies an oracle inequality like Eq. (2) with  $K_n = \mathcal{O}(1)$  as  $n$  tends to infinity?



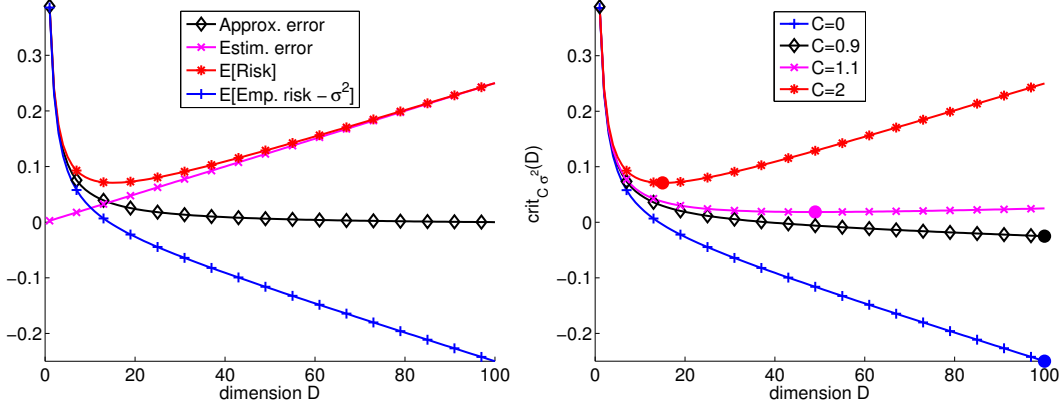


FIGURE 1. *Left: Expectations of the risk and empirical risk, bias-variance decomposition of the risk. Right:  $\text{crit}_{C\sigma^2}(m)$ , defined by Eq. (11), for  $C \in \{0, 0.9, 1.1, 2\}$ ; its minimal value at  $m^*(C\sigma^2)$  is shown by a plain dot. ‘Easy setting’, see Appendix D for detailed information.*

In order to understand how  $\hat{m}(C)$  behaves as a function of  $C$ , let us consider, for every  $C \geq 0$ ,

$$m^*(C) \in \underset{m \in \mathcal{M}}{\text{argmin}} \left\{ \mathbb{E} \left[ \frac{1}{n} \left\| \hat{F}_m - Y \right\|^2 + C \frac{D_m}{n} \right] \right\} = \underset{m \in \mathcal{M}}{\text{argmin}} \{ \text{crit}_C(m) \}$$

$$\text{with } \text{crit}_C(m) := \frac{1}{n} \left[ \left\| (I_n - \Pi_m) F \right\|^2 + (C - \sigma^2) D_m \right], \quad (11)$$

by Eq. (8). Provided that we can prove some uniform concentration inequalities for  $\|\hat{F}_m - Y\|^2$ ,  $m \in \mathcal{M}$ , we can expect  $m^*(C)$  to be close to  $\hat{m}(C)$ . Let us assume that for  $D_m$  large enough the approximation error  $n^{-1} \|(I_n - \Pi_m) F\|^2$  is almost constant. For simplicity, let us also assume that the approximation error is a decreasing function of  $D_m$ —which holds for instance if the  $S_m$  are nested. Then, two cases can be distinguished with respect to  $C$ :

- if  $C < \sigma^2$ , then  $\text{crit}_C(m)$  is a decreasing function of  $D_m$ , and  $D_{m^*(C)}$  is huge:  $m^*(C)$  overfits.
- if  $C > \sigma^2$ , then  $\text{crit}_C(m)$  increases with  $D_m$  for  $D_m$  large enough, so  $D_{m^*(C)}$  is much smaller.

This behavior is illustrated on the right part of Figure 1. In other words,

$$\text{pen}_{\min}(m) := \frac{\sigma^2 D_m}{n} \quad (12)$$

seems to be the minimal amount of penalization needed so that a minimizer  $\hat{m}$  of the penalized criterion (3) does not clearly overfit. The above arguments are made rigorous in Section 2.5, showing that  $\sigma^2 D_m/n$  is indeed a minimal penalty in the current framework.

We can now summarize the slope heuristics into two major facts. First, from Eq. (9) and (12), we get a *relationship between the optimal and minimal penalties*:

$$\text{pen}_{\text{opt}}(m) = 2 \text{pen}_{\min}(m). \quad (13)$$

Second, *the minimal penalty is observable*, since  $D_{\hat{m}(C)}$  decreases “smoothly” as a function of  $C$  everywhere except around  $C = \sigma^2$  where it jumps.

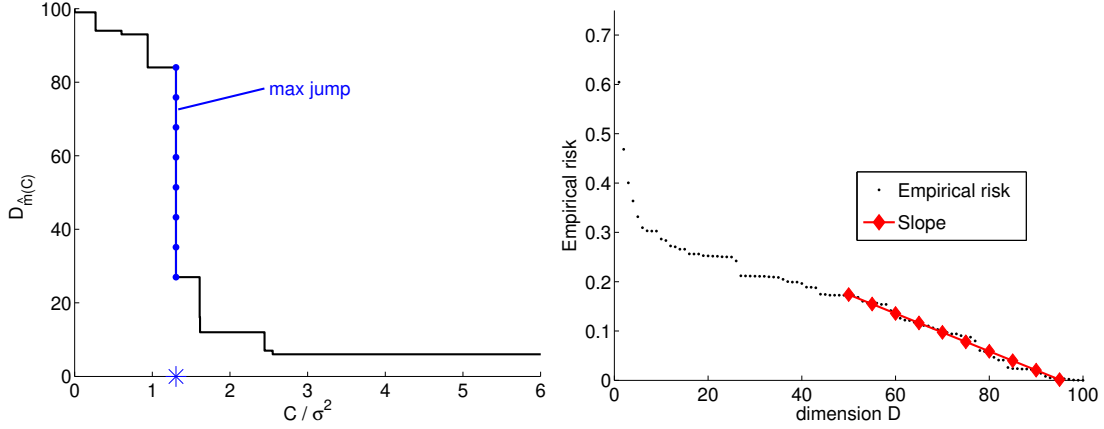


FIGURE 2. Illustration of Algorithms 1 and 2 on the same sample ('easy' setting, see Appendix D for details). Left: Plot of  $C \mapsto D_{\hat{m}(C)}$  and visualization of  $\hat{C}_{\text{jump}}$ . Right: Plot of  $D_m \mapsto n^{-1}\|Y - \hat{F}_m\|^2$  and visualization of  $-\hat{C}_{\text{slope}}/n$ .

## 2.4. Data-driven penalty algorithm

The two major facts of the slope heuristics described above directly lead to a data-driven penalization algorithm, which can be formalized in two ways.

### 2.4.1. Dimension jump

First, we can estimate the minimal penalty by looking for a jump of  $C \mapsto D_{\hat{m}(C)}$ , and make use of Eq. (13) to get an estimator of the optimal penalty.

**Algorithm 1** (Slope-heuristics algorithm, jump formulation). Input:  $(\|\hat{F}_m - Y\|^2)_{m \in \mathcal{M}}$ .

1. Compute  $(\hat{m}(C))_{C \geq 0}$ , where  $\hat{m}(C)$  is defined by Eq. (10).
2. Find  $\hat{C}_{\text{jump}} > 0$  corresponding to the "unique large jump" of  $C \mapsto D_{\hat{m}(C)}$ .
3. Select  $\hat{m}_{\text{Alg.1}} \in \operatorname{argmin}_{m \in \mathcal{M}} \{n^{-1}\|\hat{F}_m - Y\|^2 + 2\hat{C}_{\text{jump}}D_m/n\}$ .

Output:  $\hat{m}_{\text{Alg.1}}$ .

The left part of Figure 2 shows one instance of the plot of  $C \mapsto D_{\hat{m}(C)}$ , with one clear jump corresponding to  $\hat{C}_{\text{jump}}$ . Computational issues are discussed in Section 7.2; in particular, step 1 of Algorithm 1 can be done efficiently, see Appendix B.1. Step 2 of Algorithm 1 can be done in several ways, see Section 7.1. The practical problems arising with step 2 of Algorithm 1 can motivate the use of an alternative algorithm that we detail below.

### 2.4.2. Slope estimation

As explained in Section 2.3, the reason why  $D_{\hat{m}(C)}$  jumps around  $C \approx \sigma^2$  is that by Eq. (8),

$$\frac{1}{n} \mathbb{E} \left[ \left\| \hat{F}_m - Y \right\|^2 \right] = \frac{a(m) - \sigma^2 D_m}{n}$$

where  $a(m) := \|(I_n - \Pi_m)F\|^2 + n\sigma^2$ . Let us assume that  $a(m)$  —or equivalently, the approximation error— is almost constant for all  $m$  such that  $D_m$  is large enough. Then, considering only models with a large dimension, the empirical risk approximately has a linear behavior as a function of  $D_m$ , with slope  $-\sigma^2/n$ . Since the empirical risk is observable, one can estimate this slope in order to get an estimator of  $\sigma^2$ , and plug it in the optimal penalty given by Eq. (9).

**Algorithm 2** (Slope-heuristics algorithm, slope formulation). Input:  $(\|\widehat{F}_m - Y\|^2)_{m \in \mathcal{M}}$ .

1. Estimate the slope  $\widehat{S}$  of  $\|\widehat{F}_m - Y\|^2$  as a function of  $D_m$  for all  $m \in \mathcal{M}$  with  $D_m$  “large enough”, for instance by (robust) linear regression, and define  $\widehat{C}_{\text{slope}} = -n\widehat{S}$ .
2. Select  $\widehat{m}_{\text{Alg.2}} \in \operatorname{argmin}_{m \in \mathcal{M}} \{n^{-1}\|\widehat{F}_m - Y\|^2 + 2\widehat{C}_{\text{slope}}D_m/n\}$ .

Output:  $\widehat{m}_{\text{Alg.2}}$ .

The right part of Figure 2 shows an instance of the plot of  $n^{-1}\|\widehat{F}_m - Y\|^2$  as a function of  $D_m$ . Algorithm 2 relies on the choice of what is a “large enough” dimension, on how the slope  $\widehat{C}_{\text{slope}}$  is estimated, and on the assumption that the approximation error is almost constant among large models —otherwise it can fail strongly, as shown in Section 7.1. Therefore, Algorithms 1 and 2 both have pros and cons, and there is no universal choice between them. The links between Algorithms 1 and 2, as well as their differences, are discussed in Section 7.1.

## 2.5. What can be proved mathematically

A major interest of the slope heuristics is that it can be made rigorous. For instance, we prove in Section 2.7 the next theorem.

**Theorem 1.** *In the framework described in Section 2.1, assume that  $\mathcal{M}$  is finite, contains at least one model of dimension at most  $n/20$ , and that*

$$\begin{aligned} \exists m_1 \in \mathcal{M}, \quad S_{m_1} &= \mathbb{R}^n && \text{(HId)} \\ \text{and} \quad \varepsilon &\sim \mathcal{N}(0, \sigma^2 I_n). && \text{(HG)} \end{aligned}$$

Recall that for every  $C \geq 0$ ,  $\widehat{m}(C)$  is defined by Eq. (10). Then, for every  $\gamma \geq 0$ , some  $n_0(\gamma)$  exists such that if  $n \geq n_0(\gamma)$ , with probability at least  $1 - 4 \operatorname{card}(\mathcal{M})n^{-\gamma}$ , the following inequalities hold simultaneously:

$$\forall C \leq (1 - \eta_n^-) \sigma^2, \quad D_{\widehat{m}(C)} \geq \frac{9n}{10}, \quad (14)$$

$$\forall C \leq (1 - \eta_n^-) \sigma^2, \quad \frac{1}{n} \left\| \widehat{F}_{\widehat{m}(C)} - F \right\|^2 \geq \frac{7\sigma^2}{8}, \quad (15)$$

$$\forall C \geq (1 + \eta_n^+) \sigma^2, \quad D_{\widehat{m}(C)} \leq \frac{n}{10}, \quad (16)$$

$$\forall C > \sigma^2, \quad \frac{1}{n} \left\| \widehat{F}_{\widehat{m}(C)} - F \right\|^2 \leq h \left( \frac{C}{\sigma^2} \right) \left[ \inf_{m \in \mathcal{M}} \left\{ \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 \right\} + \frac{20\sigma^2 \gamma \log(n)}{n} \right], \quad (17)$$

and for every  $\eta \in (0, 1/2]$  and  $C \in [(2 - \eta)\sigma^2, (2 + \eta)\sigma^2]$ ,

$$\frac{1}{n} \left\| \widehat{F}_{\widehat{m}(C)} - F \right\|^2 \leq (1 + 3\eta) \inf_{m \in \mathcal{M}} \left\{ \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 \right\} + \frac{880\sigma^2 \gamma \log(n)}{\eta n}, \quad (18)$$

$$\text{where } \sigma^2 \eta_n^+ = 40 \inf_{m \in \mathcal{M} / D_m \leq n/20} \left\{ \frac{1}{n} \left\| (I_n - \Pi_m)F \right\|^2 \right\} + 82\sigma^2 \sqrt{\frac{\gamma \log(n)}{n}},$$

$$\eta_n^- = 41 \sqrt{\frac{\gamma \log(n)}{n}}, \quad \text{and } \forall u > 1, h(u) = \frac{10}{(u-1)^4} \mathbb{1}_{u \in (1,2)} + u^3 \mathbb{1}_{u \geq 2}.$$

Theorem 1 revisits results first obtained by [Birgé and Massart \(2007\)](#), formulating them similarly to [Arlot and Bach \(2011\)](#) but with milder assumptions.

**What Theorem 1 proves about Algorithms 1–2** Eq. (14) and (16) do not show exactly that there is a single large jump in  $C \mapsto D_{\widehat{m}(C)}$ , as in the heuristic reasoning of Section 2.3. We cannot hope to prove it since numerical experiments show that the global jump of  $D_{\widehat{m}(C)}$  can be split into several small jumps within a small interval of values of  $C$ , see Figure 5 in Section 7.1. Nevertheless, Eq. (14) and (16) imply that the variation of  $D_{\widehat{m}(C)}$  over a geometric window of  $C$  is extremely strong around  $\sigma^2$ : if  $\widehat{C}_{\text{jump}}$  in Algorithm 1 is defined as

$$\widehat{C}_{\text{window}} = \widehat{C}_{\text{window}}(\eta) \in \operatorname{argmax}_{C > 0} \{D_{\widehat{m}(C/[1+\eta])} - D_{\widehat{m}(C[1+\eta])}\} \quad (19)$$

with  $\eta = \max\{\eta_n^-, \eta_n^+\}$ , then  $\widehat{C}_{\text{window}}$  is close to  $\sigma^2$ —see Proposition 3 in Section 6.1 for a precise statement—, and Eq. (18) implies a first-order optimal oracle inequality for the model-selection procedure of Algorithm 1. Note that  $\widehat{C}_{\text{window}}$  can be computed efficiently, see Section 7.2 and Appendix B.2. In addition, Eq. (14) and (16) imply that

$$\widehat{C}_{\text{thr.}} = \widehat{C}_{\text{thr.}}(T_n) := \inf\{C \geq 0 / D_{\widehat{m}(C)} \leq T_n\} \quad (20)$$

is close to  $\sigma^2$  when  $T_n \in [n/10, 9n/10]$ —precise statements are provided by Proposition 3 in Section 6.1—, and Eq. (18) implies a first-order optimal oracle inequality for the corresponding model-selection procedure. See Section 7.1 for practical comments about these variants of Algorithm 1.

Theorem 1 does not prove that Algorithm 2 works, and it seems difficult to prove such a result without adding some assumptions. Indeed, the key heuristics behind Algorithm 2 is a linear behavior of the empirical risk as a function of the dimension, at least for large models. In the proof of Theorem 1, we control the deviations of the empirical risk around its expectation, but this is not sufficient for justifying Algorithm 2 without a *strong uniform control on the approximation errors* of the models, an assumption much stronger than the ones of Theorem 1.

Note finally that Eq. (15) and (17) are not necessary for justifying Algorithm 1, but they are interesting for theory since they justify the term “minimal penalty”. Eq. (15) is a straightforward consequence of Eq. (14), and results like Eq. (17) are easier to obtain than Eq. (18), see Section 4.4.

**Variante of Theorem 1** If  $\mathcal{M}$  contains at least one model of dimension at most  $c_n \in [0, n)$ , on the event defined in Theorem 1, we can actually prove that more results hold true: we can change Eq. (14) and (16) respectively into

$$\forall a_n < n, \quad \forall C \leq [1 - \eta_n^-(a_n)] \sigma^2, \quad D_{\hat{m}(C)} \geq a_n \quad (21)$$

$$\forall b_n > c_n, \quad \forall C \geq [1 + \eta_n^+(b_n, c_n)] \sigma^2, \quad D_{\hat{m}(C)} \leq b_n \quad (22)$$

where

$$\sigma^2 \eta_n^+(b_n, c_n) := \frac{n}{b_n - c_n} \left( 2\mathcal{B}(c_n) + 4.1 \sigma^2 \sqrt{\frac{\gamma \log(n)}{n}} \right),$$

$$\mathcal{B}(c_n) := \inf_{m \in \mathcal{M} / D_m \leq c_n} \left\{ \frac{1}{n} \|(I_n - \Pi_m)F\|^2 \right\}, \quad \text{and} \quad \eta_n^-(a_n) := 4.1 \left( 1 - \frac{a_n}{n} \right)^{-1} \sqrt{\frac{\gamma \log(n)}{n}}.$$

In particular, under the assumptions of Theorem 1, taking  $a_n \in (9n/10, n)$ ,  $b_n \in (n/20, n/10)$  and  $c_n = n/20$ , we get a larger jump of  $D_{\hat{m}(C)}$ —hence easier to detect— by considering a larger window of values of  $C$ , hence reducing the precision of the estimation of  $\sigma^2$ .

**Relaxation of the noise assumption** Assumption (HG) is a classical noise model for proving non-asymptotic oracle inequalities. In Theorem 1, it is only used for proving some concentration inequalities at the beginning of the proof—Eq. (23)–(24) in Section 2.7—, so it could be changed into any noise assumption ensuring that similar concentration inequalities hold true. For instance, Theorem 1 can be generalized to the case of sub-Gaussian noise, as formalized below.

**Remark 1** (Generalization of Theorem 1 to sub-Gaussian noise). *Assume that the  $(\varepsilon_i)_{1 \leq i \leq n}$  are centered, independent, and  $(\phi^2 \sigma^2)$ -sub-Gaussian for some  $\phi > 0$ —with any definition of sub-Gaussianity among the classical ones since they are all equivalent up to numerical constants (Boucheron et al., 2013, Section 2.3). Then, by the Cramér-Chernoff method (Boucheron et al., 2013, Section 2.2), Eq. (24) holds true with probability at least  $1 - 2 \exp(x/\phi^2)$ . In addition, Bellec (2019, Theorem 3) shows that Eq. (23) holds true with probability at least  $1 - 2 \exp[x/(L\phi^2)]$  for some numerical constant  $L$ . Therefore, the event  $\Omega_{L\phi^2 x}$  defined in the proof of Theorem 1 has a probability at least  $1 - 4 \text{card}(\mathcal{M}) e^{-x}$ . So, the result of Theorem 1 holds true with  $x$  (resp.  $\gamma$ ) replaced by  $L\phi^2 x$  (resp.  $L\phi^2 \gamma$ ) in  $n_0$ ,  $\eta_n^-$ ,  $\eta_n^+$ , and in the risk bounds (17)–(18). The same generalization holds for Eq. (21)–(22) and for consequences of Theorem 1 such as Proposition 3.*

**Comments on the assumptions on  $\mathcal{M}$**  Assumption (Hid) is barely an assumption since we can always add such a model to the collection considered (and it will never be selected by the procedure). It is used in the proof of Eq. (14) where we need to make sure that a model of large dimension and small bias exists.

Theorem 1 implicitly assumes that  $\mathcal{M}$  contains a model of dimension at most  $n/20$  with a small approximation error. This is much milder than the assumption of the corresponding results of Arlot and Bach (2009, 2011) and Arlot and Massart (2009), which is that  $\mathcal{M}$  contains a model of dimension at most  $\sqrt{n}$  with an approximation error upper bounded by  $\sigma^2 \sqrt{\log(n)/n}$ . Here, having a model of dimension  $n/20$  with approximation error  $\sigma^2/\log(n)$  is sufficient to get a consistent estimation of  $\sigma^2$  and a first-order optimal model-selection procedure. Note however

that such an assumption seems almost *necessary* for Algorithm 1 to work: if the approximation error never vanishes for a (not too) large model, and if it is not almost constant among large models—which can happen in practice—, we conjecture that the slope heuristics fails.

Finally,  $\mathcal{M}$  is assumed to be finite, but Theorem 1 implicitly assumes a little more, since the event on which the result holds has a large probability only if  $\text{card}(\mathcal{M})n^{-\gamma}$  is small, which requires to take  $\gamma$  large enough. Since  $\gamma$  appears in all the bounds, assuming that it can be chosen fixed as  $n$  grows is equivalent to assuming that  $\text{card}(\mathcal{M})$  grows at most like a power of  $n$ , which excludes model collections of exponential complexity—that is,  $\text{card}(\mathcal{M}) \propto a^n$  for some  $a > 0$ . The case of exponential collections is discussed in Sections 4.7 and 8.3.4.

## 2.6. Bibliographical remarks

**Algorithms** The slope heuristics and the corresponding data-driven penalty were first proposed by Birgé and Massart in a preprint (Birgé and Massart, 2001b) and the subsequent article (Birgé and Massart, 2007). They are also exposed by Massart (2005), Blanchard and Massart (2006, Section 2), Massart (2007, Section 8.5.2) and Massart (2008).

The term “slope” corresponds to the linear behavior of the empirical risk as a function of the dimension, as Algorithm 2 exploits.

The first implementation of data-driven penalties built upon the slope heuristics was expressed as a slope estimation, as in Algorithm 2; it was done by Letué (2000, Section A.4) for penalized maximum likelihood, inspired by a preliminary version of the preprint by Birgé and Massart (2001b).

Several practical issues with Algorithm 2 were underlined in the context of change-point detection by Lebarbier (2002, Chapter 4), who then suggested to prefer the “dimension jump” formulation of Algorithm 1 which was present in the final version of the preprint by Birgé and Massart (2001b), as well as in the articles by Massart (2005) and Birgé and Massart (2007). The drawbacks of Algorithm 1 were also underlined by Lebarbier (2002, 2005) where some automatic ways to detect the dimension jump were proposed and tested on some synthetic data. Later on, Baudry et al. (2012) studied more deeply the practical use of Algorithms 1 and 2, with several variants (see also Section 7). The first proposition of detecting a jump over some sliding window was made by Bontemps and Toussile (2013), who considered only a finite set of values of  $C$ ; to the best of our knowledge, the continuous formulation for  $\hat{C}_{\text{window}}$  is new, as well as the corresponding algorithm in Appendix B.2.

**Theory** The first theoretical results about the slope heuristics were proved in the setting of the present section, that is, regression on a fixed design with the least-squares risk and projection (least-squares) estimators. In the articles by Birgé and Massart (2001b, 2007), the first results obtained were similar to Eq. (14), (15), (17), and (18), making slightly stronger assumptions. A result similar to Eq. (15) was even published previously by Birgé and Massart (2001a), but only in the restrictive case  $F = 0$ .

The first result showing the existence of a jump—that is, Eq. (14) and (16) holding simultaneously for all  $C$  on the same large-probability event—was obtained for least-squares regression on a random design with regressogram estimators (Arlot and Massart, 2009). It was then proved

in the fixed-design setting with more general estimators including projection estimators (Arlot and Bach, 2009, 2011).

Eq. (17) is a corollary of a classical non-asymptotic oracle inequality for  $C_p$ -like penalties; similar results were known before the introduction of the slope heuristics (see for instance Barron et al., 1999). Eq. (18) is more precise because of the constant  $1 + o(1)$  in front of the oracle risk, which was first obtained by Birgé and Massart (2001b, 2007).

The extension of Theorem 1 to sub-Gaussian noise (Remark 1 in Section 2.5) is new, to the best of our knowledge.

## 2.7. Proof of Theorem 1

The proof mixes ideas from Birgé and Massart (2007) and Arlot and Bach (2011). We split it into three main steps, the last two ones being split themselves into several substeps: (1) using concentration inequalities, (2) proving the existence of a dimension jump (Eq. (14)–(16)), and (3) proving risk bounds thanks to a general oracle inequality (Eq. (17)–(18)).

We define  $n_0(\gamma)$  as the smallest integer such that  $\gamma \log(n)/n \leq 1/80^2$  for every  $n \geq n_0(\gamma)$ . At various places in the proof (in steps 2.3, 3.2, and 3.3), we make use of the inequality: for all  $a, b, \theta > 0$ ,  $2\sqrt{ab} \leq \theta a + \theta^{-1}b$ .

**Step 1: concentration inequalities** As explained in Section 2.3, the slope heuristics relies on the fact that  $\|\widehat{F}_m - Y\|^2$  is close to its expectation. Let  $x \geq 0$  be fixed. Given Eq. (5)–(6), for every  $m \in \mathcal{M}$ , we consider the event  $\Omega_{m,x}$  on which the following two inequalities hold simultaneously:

$$|\langle \varepsilon, \Pi_m \varepsilon \rangle - \sigma^2 D_m| \leq 2\sigma^2 \sqrt{x D_m} + 2x\sigma^2 \quad (23)$$

$$|\langle \varepsilon, (I_n - \Pi_m)F \rangle| \leq \sigma \sqrt{2x} \|(I_n - \Pi_m)F\|. \quad (24)$$

Under (HG), by standard Gaussian concentration results (for instance, Arlot and Bach, 2011, Propositions 4 and 6)—, we have

$$\mathbb{P}(\Omega_{m,x}) \geq 1 - 4e^{-x}.$$

Then, defining  $\Omega_x := \bigcap_{m \in \mathcal{M}} \Omega_{m,x}$ , the union bound gives

$$\mathbb{P}(\Omega_x) \geq 1 - 4 \text{card}(\mathcal{M}) e^{-x}$$

and it is sufficient to prove that Eq. (14)–(18) hold true on  $\Omega_x$  with  $x = \gamma \log(n)$ .

From now on, we restrict ourselves to the event  $\Omega_x$ .

**Step 2: existence of a dimension jump** For proving Eq. (14) and (16), we show that  $\widehat{m}(C)$  minimizes a quantity  $G_C(m)$  close to  $\text{crit}_C(m)$ , and then we show that  $G_C(m_1)$  (resp.  $G_C(m_2)$ ), for some well-chosen  $m_2 \in \mathcal{M}$  is smaller than  $G_C(m)$  for any model  $m$  with  $D_m < 9n/10$  (resp.  $D_m > n/10$ ).



**Step 2.1: control of the difference between  $\text{crit}_C(m)$  and the quantity minimized by  $\widehat{m}(C)$**   
 Let  $C \geq 0$ . By Eq. (10), (5), and (6), since  $\|\varepsilon\|^2$  does not depend from  $m$ ,  $\widehat{m}(C)$  minimizes over  $\mathcal{M}$  the function  $G_C : \mathcal{M} \rightarrow \mathbb{R}$  defined by

$$\begin{aligned} \forall m \in \mathcal{M}, \quad G_C(m) &:= \frac{1}{n} \left\| \widehat{F}_m - Y \right\|^2 + C \frac{D_m}{n} - \frac{1}{n} \|\varepsilon\|^2 \\ &= \frac{1}{n} \left\| (I_n - \Pi_m)F \right\|^2 - \frac{1}{n} \langle \varepsilon, \Pi_m \varepsilon \rangle + C \frac{D_m}{n} + \frac{2}{n} \langle \varepsilon, (I_n - \Pi_m)F \rangle \\ &= \text{crit}_C(m) - \left( \frac{1}{n} \langle \varepsilon, \Pi_m \varepsilon \rangle - \sigma^2 D_m \right) + \frac{2}{n} \langle \varepsilon, (I_n - \Pi_m)F \rangle \end{aligned}$$

where  $\text{crit}_C$  is defined by Eq. (11). Therefore, by Eq. (23)–(24) and using  $D_m \leq n$ , for every  $m \in \mathcal{M}$ ,

$$|G_C(m) - \text{crit}_C(m)| \leq 2\sigma^2 \left( \sqrt{\frac{x}{n}} + \frac{x}{n} \right) + \frac{2\sigma\sqrt{2x}}{n} \|(I_n - \Pi_m)F\|. \quad (25)$$

**Step 2.2: lower bound on  $D_{\widehat{m}(C)}$  when  $C$  is too small (proof of Eq. (14))** Let  $C \in [0, \sigma^2)$ . Since  $\widehat{m}(C)$  minimizes  $G_C(m)$  over  $m \in \mathcal{M}$ , it is sufficient to prove that if  $C \leq (1 - \eta_n^-)\sigma^2$ ,

$$G_C(m_1) < \inf_{m \in \mathcal{M}, D_m < 9n/10} \{G_C(m)\} \quad (26)$$

where  $m_1$  is given by (HId). On the one hand, by Eq. (25),

$$G_C(m_1) \leq \text{crit}_C(m_1) + 2\sigma^2 \left( \sqrt{\frac{x}{n}} + \frac{x}{n} \right) = C - \sigma^2 + 2\sigma^2 \left( \sqrt{\frac{x}{n}} + \frac{x}{n} \right). \quad (27)$$

On the other hand, by Eq. (25), for any  $m \in \mathcal{M}$  such that  $D_m < 9n/10$ ,

$$\begin{aligned} G_C(m) &\geq \frac{(C - \sigma^2)D_m}{n} - 2\sigma^2 \left( \sqrt{\frac{x}{n}} + \frac{x}{n} \right) + \frac{1}{n} \|(I_n - \Pi_m)F\|^2 - \frac{2\sigma\sqrt{2x}}{n} \|(I_n - \Pi_m)F\| \\ &> \frac{9}{10}(C - \sigma^2) - 2\sigma^2 \left( \sqrt{\frac{x}{n}} + \frac{2x}{n} \right). \end{aligned} \quad (28)$$

To conclude, the upper bound in Eq. (27) is smaller than the lower bound in Eq. (28) when

$$C \leq \sigma^2 \left( 1 - 40\sqrt{\frac{x}{n}} - 60\frac{x}{n} \right) =: \widetilde{C}_1(x). \quad (29)$$

Taking  $x = \gamma \log(n)$ , for  $n \geq n_0(\gamma)$ , we have  $\widetilde{C}_1(x) \geq \sigma^2(1 - \eta_n^-)$  hence Eq. (14).

Remark that the same reasoning with  $9n/10$  replaced by any  $a_n \in [0, n)$  proves that  $D_{\widehat{m}(C)} \geq a_n$  for every

$$C \leq \sigma^2 \left( 1 - \frac{4\sqrt{\frac{x}{n}} + 6\frac{x}{n}}{1 - \frac{a_n}{n}} \right) =: C_1(x; a_n). \quad (30)$$

We get Eq. (21) by taking  $x = \gamma \log(n)$  and using that  $x/n \leq 1/60^2$  since  $n \geq n_0(\gamma)$ .



**Step 2.3: upper bound on  $D_{\hat{m}(C)}$  when  $C$  is large enough (proof of Eq. (16))** Let  $C > \sigma^2$ . Similarly to the proof of Eq. (14), it is sufficient to prove that if  $C \geq (1 + \eta_n^+) \sigma^2$ ,

$$G_C(m_2) < \inf_{m \in \mathcal{M}, D_m > n/10} \{G_C(m)\} \quad (31)$$

where  $m_2 \in \operatorname{argmin}_{m \in \mathcal{M} / D_m \leq n/20} \{\|(I_n - \Pi_m)F\|^2\}$  exists by assumption. For any  $c_n \in [0, n]$ , let us define

$$\mathcal{B}(c_n) := \inf_{m \in \mathcal{M} / D_m \leq c_n} \left\{ \frac{1}{n} \|(I_n - \Pi_m)F\|^2 \right\},$$

so that  $m_2$  has an approximation error equal to  $\mathcal{B}(n/20)$ . On the one hand, by Eq. (25),

$$\begin{aligned} G_C(m_2) &\leq \operatorname{crit}_C(m_2) + 2\sigma^2 \left( \sqrt{\frac{x}{n} + \frac{x}{n}} \right) + \frac{2\sigma\sqrt{2x}}{n} \|(I_n - \Pi_{m_2})F\| \\ &\leq \frac{2}{n} \|(I_n - \Pi_{m_2})F\|^2 + \frac{(C - \sigma^2)D_{m_2}}{n} + 2\sigma^2 \left( \sqrt{\frac{x}{n} + \frac{2x}{n}} \right) \\ &\leq 2\mathcal{B}\left(\frac{n}{20}\right) + (C - \sigma^2) \frac{n/20}{n} + 2\sigma^2 \left( \sqrt{\frac{x}{n} + \frac{2x}{n}} \right). \end{aligned} \quad (32)$$

On the other hand, by Eq. (25), for any  $m \in \mathcal{M}$  such that  $D_m > n/10$ ,

$$G_C(m) > \frac{n/10}{n} (C - \sigma^2) - 2\sigma^2 \left( \sqrt{\frac{x}{n} + \frac{2x}{n}} \right). \quad (33)$$

To conclude, the upper bound in Eq. (32) is smaller than the lower bound in Eq. (33) when

$$C \geq \sigma^2 \left[ 1 + 80 \left( \sqrt{\frac{x}{n} + \frac{2x}{n}} \right) \right] + 40\mathcal{B}\left(\frac{n}{20}\right) =: \tilde{C}_2(x). \quad (34)$$

Taking  $x = \gamma \log(n)$ , for  $n \geq n_0(\gamma)$ , we have  $\tilde{C}_2(x) \leq \sigma^2(1 + \eta_n^+)$  hence Eq. (16).

Remark that if  $\mathcal{M}$  contains a model of dimension at most  $c_n \in [0, n]$ , the same reasoning with  $n/10$  replaced by any  $b_n \in (c_n, n]$  and  $n/20$  replaced by  $c_n$  proves that  $D_{\hat{m}(C)} \leq b_n$  for every

$$C \geq \sigma^2 \left[ 1 + \frac{4n}{b_n - c_n} \left( \sqrt{\frac{x}{n} + \frac{2x}{n}} \right) \right] + \frac{2n}{b_n - c_n} \mathcal{B}(c_n) =: C_2(x; b_n; c_n). \quad (35)$$

We get Eq. (22) by taking  $x = \gamma \log(n)$  and using that  $x/n \leq 1/80^2$  since  $n \geq n_0(\gamma)$ .

Until the end of the proof, we fix  $x = \gamma \log(n)$ .

**Step 2.4: lower bound on the risk of large models (proof of Eq. (15))** This is a straightforward consequence of Eq. (14). Indeed, on  $\Omega_x$ , for any  $m \in \mathcal{M}$  such that  $D_m \geq 9n/10$ ,

$$\begin{aligned} \frac{1}{n} \|F - \hat{F}_m\|^2 &= \frac{1}{n} \|(I_n - \Pi_m)F\|^2 + \frac{1}{n} \langle \varepsilon, \Pi_m \varepsilon \rangle \\ &\geq \frac{\sigma^2}{n} (D_m - 2\sqrt{x}D_m - 2x) = \frac{\sigma^2}{n} \left[ (\sqrt{D_m} - \sqrt{x})^2 - 3x \right] \geq \frac{7\sigma^2}{8}, \end{aligned}$$

where we use that  $x/n \leq 1/77^2$  since  $n \geq n_0(\gamma)$ .

**Step 3: upper bounds on the risk** For proving Eq. (17)–(18), we prove a slightly more general oracle inequality —Eq. (43)— using the classical approach used for instance by [Birgé and Massart \(2001a\)](#), [Massart \(2007\)](#) and [Arlot and Bach \(2011\)](#).

**Step 3.1: general approach for proving an oracle inequality** Following Section 2.2, an ideal penalty is

$$\text{pen}_{\text{id}}(m) := \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 - \frac{1}{n} \left\| \widehat{F}_m - Y \right\|^2 + \|\varepsilon\|^2$$

which has expectation  $2\sigma^2 D_m/n = \text{pen}_{\text{opt}}(m)$ . A key argument for getting an oracle inequality is that  $\text{pen}_{\text{id}}(m)$  concentrates around its expectation. Indeed, let us define

$$\Delta(m) := \text{pen}_{\text{id}}(m) - \frac{2\sigma^2 D_m}{n} = \frac{2}{n} \left( \langle \varepsilon, \Pi_m \varepsilon \rangle - \sigma^2 D_m \right) - \frac{2}{n} \langle \varepsilon, (I_n - \Pi_m)F \rangle, \quad (36)$$

where the second formulation is a consequence of Eq. (6). Then, by Eq. (10), for any  $C \geq 0$  and  $m \in \mathcal{M}$ ,

$$\frac{1}{n} \left\| \widehat{F}_{\widehat{m}(C)} - Y \right\|^2 + \frac{CD_{\widehat{m}(C)}}{n} \leq \frac{1}{n} \left\| \widehat{F}_m - Y \right\|^2 + \frac{CD_m}{n}$$

which is equivalent to

$$\frac{1}{n} \left\| \widehat{F}_{\widehat{m}(C)} - F \right\|^2 - \Delta(\widehat{m}(C)) + \frac{(C - 2\sigma^2)D_{\widehat{m}(C)}}{n} \leq \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 - \Delta(m) + \frac{(C - 2\sigma^2)D_m}{n}. \quad (37)$$

It remains to show that  $\Delta(m)$  and  $(C - 2\sigma^2)D_m/n$  are small compared to  $n^{-1} \left\| \widehat{F}_m - F \right\|^2$  for all  $m \in \mathcal{M}$ . Recall that we restrict ourselves to the event  $\Omega_x$  until the end of the proof, with  $x = \gamma \log(n)$ .

**Step 3.2: control of  $\Delta(m)$**  By Eq. (23), (24), and (36), for every  $m \in \mathcal{M}$  and  $\theta > 0$ ,

$$\begin{aligned} |\Delta(m)| &\leq \frac{2}{n} \left[ 2\sigma^2 \sqrt{x D_m} + 2\sigma^2 x + \sigma \sqrt{2x} \left\| (I_n - \Pi_m)F \right\| \right] \\ &\leq 2\theta \mathbb{E} \left[ \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 \right] + \frac{\sigma^2 x}{n} (3\theta^{-1} + 4). \end{aligned} \quad (38)$$

**Step 3.3: upper bound on the expected risk in terms of risk** By Eq. (5) and (24), for every  $m \in \mathcal{M}$  and  $\theta' > 0$ ,

$$\begin{aligned} \left\| \widehat{F}_m - F \right\|^2 &= \mathbb{E} \left[ \left\| \widehat{F}_m - F \right\|^2 \right] + \langle \varepsilon, \Pi_m \varepsilon \rangle - \sigma^2 D_m \\ &\geq \mathbb{E} \left[ \left\| \widehat{F}_m - F \right\|^2 \right] - \sigma^2 (2\sqrt{x D_m} + 2x) \\ &\geq (1 - \theta') \mathbb{E} \left[ \left\| \widehat{F}_m - F \right\|^2 \right] - x\sigma^2 (2 + \theta'^{-1}) \end{aligned}$$

so that, for every  $\theta' \in (0, 1)$ ,

$$\mathbb{E} \left[ \left\| \widehat{F}_m - F \right\|^2 \right] \leq \frac{1}{1 - \theta'} \left\| \widehat{F}_m - F \right\|^2 + \kappa(\theta') x \sigma^2 \quad \text{with} \quad \kappa(\theta') := \frac{2 + \frac{1}{\theta'}}{1 - \theta'}. \quad (39)$$

**Step 3.4: control of the remainder terms appearing in Eq. (37)** Combining Eq. (38) and (39), we get on the one hand that for every  $m \in \mathcal{M}$ ,  $\theta > 0$ ,  $\theta' \in (0, 1)$ ,

$$\begin{aligned} & \Delta(m) + \frac{(2\sigma^2 - C)D_m}{n} \\ & \leq \left[ 2\theta + \left( 2 - \frac{C}{\sigma^2} \right)_+ \right] \mathbb{E} \left[ \frac{1}{n} \|\widehat{F}_m - F\|^2 \right] + \frac{\sigma^2 x}{n} \left( \frac{3}{\theta} + 4 \right) \\ & \leq \frac{2\theta + \left( 2 - \frac{C}{\sigma^2} \right)_+}{1 - \theta'} \frac{1}{n} \|\widehat{F}_m - F\|^2 + \frac{\sigma^2 x}{n} \left( \frac{3}{\theta} + 4 + \kappa(\theta') \left[ 2\theta + \left( 2 - \frac{C}{\sigma^2} \right)_+ \right] \right). \end{aligned} \quad (40)$$

On the other hand, similarly, for every  $m \in \mathcal{M}$ ,  $\theta > 0$ ,  $\theta' \in (0, 1)$ ,

$$\begin{aligned} & -\Delta(m) + \frac{(C - 2\sigma^2)D_m}{n} \\ & \leq \frac{2\theta + \left( \frac{C}{\sigma^2} - 2 \right)_+}{1 - \theta'} \frac{1}{n} \|\widehat{F}_m - F\|^2 + \frac{\sigma^2 x}{n} \left( \frac{3}{\theta} + 4 + \kappa(\theta') \left[ 2\theta + \left( \frac{C}{\sigma^2} - 2 \right)_+ \right] \right). \end{aligned} \quad (41)$$

**Step 3.5: proof of a general oracle inequality** Combining Eq. (37), (40), and (41) above with  $\theta' = 2\theta \in (0, 1)$ , we get that for every  $\theta \in (0, 1/2)$  and  $m \in \mathcal{M}$ ,

$$\begin{aligned} & \left[ 1 - \frac{2\theta + \left( 2 - \frac{C}{\sigma^2} \right)_+}{1 - 2\theta} \right] \frac{1}{n} \|\widehat{F}_{\widehat{m}(C)} - F\|^2 \\ & \leq \left[ 1 + \frac{2\theta + \left( \frac{C}{\sigma^2} - 2 \right)_+}{1 - 2\theta} \right] \frac{1}{n} \|\widehat{F}_m - F\|^2 + \frac{\sigma^2 x}{n} R_1(\theta, C\sigma^{-2}) \end{aligned} \quad (42)$$

$$\text{with } R_1(\theta, C\sigma^{-2}) := \frac{6}{\theta} + 8 + \kappa(2\theta) \left( 4\theta + \left| \frac{C}{\sigma^2} - 2 \right| \right).$$

Let us assume  $C > \sigma^2$ . For any  $\delta \in (0, 1]$ , we choose

$$\theta = \theta^*(\delta, C\sigma^{-2}) := \frac{\delta}{4} \frac{\left[ 1 - \left( 2 - \frac{C}{\sigma^2} \right)_+ \right]^2}{1 + \left( \frac{C}{\sigma^2} - 2 \right)_+ + \delta \left[ 1 - \left( 2 - \frac{C}{\sigma^2} \right)_+ \right]} < \frac{\delta}{4} \leq \frac{1}{4}.$$

So, if  $C \geq (1 + \delta)\sigma^2$ , we have  $C > (1 + 4\theta)\sigma^2$  hence we can divide both sides of Eq. (42) by

$$1 - \frac{2\theta + \left( 2 - \frac{C}{\sigma^2} \right)_+}{1 - 2\theta} > 0.$$

Remark that

$$\left[ 1 + \frac{2\theta + \left( \frac{C}{\sigma^2} - 2 \right)_+}{1 - 2\theta} \right] \times \left[ 1 - \frac{2\theta + \left( 2 - \frac{C}{\sigma^2} \right)_+}{1 - 2\theta} \right]^{-1} = \frac{1 + \left( \frac{C}{\sigma^2} - 2 \right)_+}{1 - 4\theta - \left( 2 - \frac{C}{\sigma^2} \right)_+} = \frac{1 + \left( \frac{C}{\sigma^2} - 2 \right)_+}{1 - \left( 2 - \frac{C}{\sigma^2} \right)_+} + \delta$$

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where the last equality uses  $\theta = \theta^*(\delta, C\sigma^{-2})$ . So, if  $C \geq (1 + \delta)\sigma^2$ , Eq. (42) leads to

$$\frac{1}{n} \left\| \widehat{F}_{\widehat{m}(C)} - F \right\|^2 \leq \left( \frac{1 + \left(\frac{C}{\sigma^2} - 2\right)_+}{1 - \left(2 - \frac{C}{\sigma^2}\right)_+} + \delta \right) \left[ \inf_{m \in \mathcal{M}} \left\{ \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 \right\} + \frac{\sigma^2 x}{n} R_2 \left( \delta, \frac{C}{\sigma^2} \right) \right] \quad (43)$$

where for every  $\delta \in (0, 1]$  and  $u \in (1, +\infty)$ ,

$$R_2(\delta, u) = R_1(\theta^*(\delta, u), u) \leq (10 + 2|u - 2|)\theta^*(\delta, u)^{-1}.$$

Therefore, for every  $C \geq (1 + \delta)\sigma^2$ ,

$$R_2 \left( \delta, \frac{C}{\sigma^2} \right) \leq \frac{8}{\delta} (5 + |C\sigma^{-2} - 2|) \max \left\{ 2 + (C\sigma^{-2} - 2)_+, \frac{2}{[1 - (2 - C\sigma^{-2})_+]^2} \right\}.$$

**Step 3.6: risk bound for  $\widehat{m}(C)$  when  $C$  is large enough (proof of Eq. (17))** In this step, we assume  $C > \sigma^2$ . When  $C/\sigma^2 \in (1, 2]$ , Eq. (43) with  $\delta = C\sigma^{-2} - 1 \in (0, 1]$  yields

$$\frac{1}{n} \left\| \widehat{F}_{\widehat{m}(C)} - F \right\|^2 \leq 2 \left( \frac{C}{\sigma^2} - 1 \right)^{-1} \left[ \inf_{m \in \mathcal{M}} \left\{ \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 \right\} + \frac{96\sigma^2 x}{n} \left( \frac{C}{\sigma^2} - 1 \right)^{-3} \right].$$

When  $C/\sigma^2 \geq 2$ , Eq. (43) with  $\delta = 1$  yields

$$\frac{1}{n} \left\| \widehat{F}_{\widehat{m}(C)} - F \right\|^2 \leq \frac{C}{\sigma^2} \left[ \inf_{m \in \mathcal{M}} \left\{ \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 \right\} + \frac{20\sigma^2 x}{n} \left( \frac{C}{\sigma^2} \right)^2 \right].$$

Eq. (17) follows.

**Step 3.7: oracle inequality for  $\widehat{m}(C)$  when  $C$  is close to  $2\sigma^2$  (proof of Eq. (18))** Now, we assume  $C/\sigma^2 \in [2 - \eta, 2 + \eta]$  with  $\eta \in [0, 1/2]$ . Taking  $\delta = \eta$  in Eq. (43) yields

$$\begin{aligned} \frac{1}{n} \left\| \widehat{F}_{\widehat{m}(C)} - F \right\|^2 &\leq \left( \max \left\{ 1 + \eta, \frac{1}{1 - \eta} \right\} + \eta \right) \\ &\quad \times \left[ \inf_{m \in \mathcal{M}} \left\{ \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 \right\} + \frac{\sigma^2 x}{n} \frac{8}{\eta} (5 + \eta) \max \left\{ 2 + \eta, \frac{2}{(1 - \eta)^2} \right\} \right] \\ &\leq (1 + 3\eta) \inf_{m \in \mathcal{M}} \left\{ \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 \right\} \\ &\quad + \frac{\sigma^2 x}{n} \frac{8}{\eta} (1 + 3\eta) (5 + \eta) \max \left\{ 2 + \eta, \frac{2}{(1 - \eta)^2} \right\} \\ &\leq (1 + 3\eta) \inf_{m \in \mathcal{M}} \left\{ \frac{1}{n} \left\| \widehat{F}_m - F \right\|^2 \right\} + \frac{880\sigma^2 x}{\eta n}, \end{aligned}$$

using that  $1/(1 - \eta) \leq 1 + 2\eta$  for every  $\eta \in [0, 1/2]$ . Eq. (18) follows.  $\square$

### 3. Generalizing the slope heuristics

The slope heuristics has first been formulated and theoretically validated in the framework of Section 2. Then, it rapidly became a more general heuristics for building data-driven optimal penalties. This section discusses two possible formulations for its generalization.

#### 3.1. General framework

Before going any further, we need to introduce a general model/estimator-selection framework. Let  $\mathbb{S}$  be some set,  $\mathcal{R} : \mathbb{S} \mapsto [0, +\infty)$  be some risk function, and assume that our goal is to build from data some estimator  $\hat{s} \in \mathbb{S}$  such that  $\mathcal{R}(\hat{s})$  is as small as possible. Let  $(\hat{s}_m)_{m \in \mathcal{M}}$  be a collection of estimators. The goal of estimator selection is to choose from data some  $\hat{m} \in \mathcal{M}$  such that the risk of  $\hat{s}_{\hat{m}}$  is as small as possible, that is, satisfying an oracle inequality

$$\mathcal{R}(\hat{s}_{\hat{m}}) - \mathcal{R}(s^*) \leq K_n \inf_{m \in \mathcal{M}} \{ \mathcal{R}(\hat{s}_m) - \mathcal{R}(s^*) \} + R_n \quad (44)$$

with large probability, where  $\mathcal{R}(s^*) := \inf_{t \in \mathbb{S}} \mathcal{R}(t)$ . In the following,  $K_n$  is called “the leading constant” of the oracle inequality (44). Let  $\hat{\mathcal{R}}_n : \mathbb{S} \mapsto [0, +\infty)$  be the empirical risk associated with  $\mathcal{R}$ , that is, we assume throughout Sections 3–5 that  $\forall t \in \mathbb{S}$ ,  $\mathbb{E}[\hat{\mathcal{R}}_n(t)] = \mathcal{R}(t)$ .

This framework includes the one of Section 2 by taking  $\mathbb{S} = \mathbb{R}^n$ ,  $\mathcal{R}(t) = n^{-1} \|t - F\|^2 + \sigma^2$ ,  $\hat{s}_m = \hat{F}_m$  the projection estimator associated with some model  $S_m$  for every  $m \in \mathcal{M}$ , and the  $L^2$  empirical risk  $\hat{\mathcal{R}}_n(t) = n^{-1} \|t - Y\|^2$ . Many other classical settings also fit into this framework, such as density estimation with the Kullback risk or the  $L^2$  risk, random-design regression with the  $L^2$  risk, and classification with the 0–1 risk (see Arlot and Celisse, 2010, Section 1, for details).

#### 3.2. Penalties known up to some constant factor

The most natural extension of the slope heuristics is to generalize it to all frameworks where a penalty is known up to some multiplicative constant (Massart, 2005; Blanchard and Massart, 2006), that is, if theoretical results show that a good penalty is  $C^* \text{pen}_1(m)$  with  $\text{pen}_1$  known but  $C^*$  unknown. Penalties known up to a constant factor appear in several frameworks, for four main reasons:

1. A penalty satisfying an optimal oracle inequality —that is, an oracle inequality with leading constant  $1 + o(1)$ — is theoretically known, but involves *unknown quantities* in practice, such as the noise-level  $\sigma^2$  for Mallows’  $C_p$  and  $C_L$  (Mallows, 1973), see Sections 2 and 3.3.
2. An optimal penalty  $\text{pen}_1$  is known theoretically and in practice, but only *asymptotically*, that is, the (unknown) non-asymptotic optimal penalty is  $C_n^* \text{pen}_1$  with  $C_n^* \rightarrow 1$  as the sample size  $n$  tends to infinity, but  $C_n^*$  is unknown and can be far from 1 for finite sample sizes. For instance, AIC (Akaike, 1973) and BIC (Schwarz, 1978) penalties for maximum likelihood rely on asymptotic computations. Section 8.4 explains why such a problem can arise in almost any framework.

3. An optimal penalty is obtained by resampling, hence depending on some multiplicative factor that might depend on unknown quantities or be correct only for  $n$  large enough, see Remark 3 in Section 4.2 and the article by Arlot (2009).
4. A penalty  $C \text{pen}_1$  satisfying an oracle inequality with a leading constant  $\mathcal{O}(1)$  when  $C$  is well chosen is known theoretically, but theoretical results are not precise enough to specify the optimal value  $C^*$  of  $C$ . This occurs for instance for change-point detection (Comte and Rozenholc, 2004; Lebarbier, 2005), density estimation with Gaussian mixtures (Maugis and Michel, 2011b), and local Rademacher complexities in classification (Bartlett et al., 2005; Koltchinskii, 2006). In some frameworks, some partial information is available about the optimal value of the constant: in binary classification, global Rademacher complexities differ by a factor 2 between theory (Koltchinskii, 2001) and practice (Lozano, 2000). Note that in such cases, it might happen that  $C^* \text{pen}_1$  is not exactly an optimal penalty, so that no oracle inequality with leading constant  $1 + o(1)$  can be obtained; nevertheless, choosing the constant  $C$  in the penalty  $C \text{pen}_1$  remains an important practical problem.

Then, if for every  $m \in \mathcal{M}$ ,  $\mathcal{C}_m$  measures the ‘‘complexity’’ of  $\hat{s}_m$ , the slope heuristics suggests to generalize Algorithm 1 into the following.

**Algorithm 3** (Slope-heuristics algorithm, jump formulation, general setting).

Input:  $(\hat{\mathcal{R}}_n(\hat{s}_m))_{m \in \mathcal{M}}$ ,  $(\text{pen}_1(m))_{m \in \mathcal{M}}$ , and  $(\mathcal{C}_m)_{m \in \mathcal{M}}$ .

1. Compute  $(\hat{m}_1(C))_{C \geq 0}$ , where for every  $C \geq 0$ ,

$$\hat{m}_1(C) \in \underset{m \in \mathcal{M}}{\text{argmin}} \left\{ \hat{\mathcal{R}}_n(\hat{s}_m) + C \text{pen}_1(m) \right\}. \quad (45)$$

2. Find  $\hat{C}_{\text{jump}} > 0$  corresponding to the ‘‘unique large jump’’ of  $C \mapsto \mathcal{C}_{\hat{m}_1(C)}$ .
3. Select  $\hat{m}_{\text{Alg.3}} \in \underset{m \in \mathcal{M}}{\text{argmin}} \left\{ \hat{\mathcal{R}}_n(\hat{s}_m) + 2\hat{C}_{\text{jump}} \text{pen}_1(m) \right\}$ .

Output:  $\hat{m}_{\text{Alg.3}}$ .

Algorithm 3 relies on two ideas: (i) Eq. (13), that is,  $\text{pen}_{\text{opt}} = 2 \text{pen}_{\text{min}}$ , is valid in a more general framework than least-squares regression and projection estimators, and (ii) if a proper complexity measure  $\mathcal{C}_m$  is used instead of the dimension  $D_m$  of the models, the minimal penalty can be characterized empirically by a jump of  $\mathcal{C}_{\hat{m}_1(C)}$ .

### 3.3. Algorithm 3 fails for linear-estimator selection

We now illustrate on an example why Algorithm 3 can fail, before showing how to correct it in Section 3.4. Let us consider the fixed-design regression framework of Section 2.1 with linear estimators instead of projection estimators, that is, for every  $m \in \mathcal{M}$ ,

$$\hat{F}_m = A_m Y$$

for some deterministic linear mapping  $A_m : \mathbb{R}^n \rightarrow \mathbb{R}^n$ . For instance, projection estimators are linear estimators since the orthogonal projection  $A_m = \Pi_m$  onto a linear space  $S_m$  is linear. Other

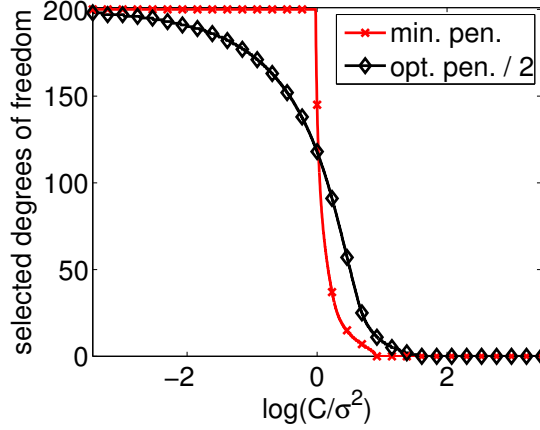


FIGURE 3. The minimal penalty is not proportional to  $\text{tr}(A_m)$  for kernel ridge estimators (Figure taken from the article by Arlot and Bach (2011), ‘kernel ridge’ framework, see Appendix D for details):  $C \mapsto \mathcal{C}_{\hat{m}_1(C)}$  for Algorithm 3 with  $\text{pen}_1(m) = \text{tr}(A_m)/n$  and  $\mathcal{C}_m = \text{tr}(A_m)$  (black curve / diamonds), and  $C \mapsto \text{tr}(A_{\hat{m}_{\min}^{\text{lin}}(C)})$  for Algorithm 4 (red curve / crosses) with linear estimators (kernel ridge).

examples include kernel ridge regression or spline smoothing, nearest-neighbor regression, and Nadaraya-Watson estimators (Arlot and Bach, 2011, provide more examples and references).

Similarly to Section 2.2, expectations of the risk and empirical risk of a linear estimator can be computed as follows:

$$\mathbb{E} \left[ \frac{1}{n} \left\| \hat{F}_m - F \right\|^2 \right] = \frac{1}{n} \left\| (I_n - A_m) F \right\|^2 + \frac{\sigma^2 \text{tr}(A_m^\top A_m)}{n}, \quad (46)$$

$$\mathbb{E} \left[ \frac{1}{n} \left\| \hat{F}_m - Y \right\|^2 \right] = \frac{1}{n} \left\| (I_n - A_m) F \right\|^2 + \frac{\sigma^2 [n + \text{tr}(A_m^\top A_m) - 2 \text{tr}(A_m)]}{n}, \quad (47)$$

$$\text{and } \text{pen}_{\text{opt}}(m) = \mathbb{E} \left[ \frac{1}{n} \left\| \hat{F}_m - F \right\|^2 \right] - \mathbb{E} \left[ \frac{1}{n} \left\| \hat{F}_m - Y \right\|^2 \right] + \sigma^2 = \frac{2\sigma^2 \text{tr}(A_m)}{n}. \quad (48)$$

Eq. (46) can be interpreted as a bias-variance decomposition similarly to Eq. (7). The optimal penalty given by Eq. (48) has been called  $C_L$  by Mallows (1973) and is similar to  $C_p$ , with the dimension  $D_m$  replaced by the *degrees of freedom*  $\text{tr}(A_m)$ . It also depends on  $\sigma^2$  which is unknown, so one could think of using Algorithm 3 with  $\hat{s}_m = \hat{F}_m$ ,  $\hat{\mathcal{R}}_n(t) = n^{-1} \|t - Y\|^2$ ,  $\text{pen}_1(m) = \text{tr}(A_m)/n$ , and  $\mathcal{C}_m = \text{tr}(A_m)$ . Then, plotting  $\mathcal{C}_{\hat{m}_1(C)}$  as a function of  $C$ , what we typically get is shown in Figure 3 (black curve / diamonds): no clear jump of the complexity is observed around  $\sigma^2$ , contrary to what Algorithm 3 predicts.

### 3.4. Minimal-penalty heuristics for linear estimators

Following Arlot and Bach (2009, 2011), the correct minimal penalty in the linear-estimators framework is

$$\text{pen}_{\min}^{\text{lin}}(m) := \frac{\sigma^2 [2 \text{tr}(A_m) - \text{tr}(A_m^\top A_m)]}{n}.$$

Indeed, as in Section 2.3, let us consider, for every  $C \geq 0$ ,

$$\begin{aligned} \widehat{m}_{\min}^{\text{lin}}(C) &\in \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \frac{1}{n} \|\widehat{F}_m - Y\|^2 + C \frac{2 \operatorname{tr}(A_m) - \operatorname{tr}(A_m^\top A_m)}{n} \right\}, \\ \text{and } m_{\min}^{\star \text{lin}}(C) &\in \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \mathbb{E} \left[ \frac{1}{n} \|\widehat{F}_m - Y\|^2 + C \frac{2 \operatorname{tr}(A_m) - \operatorname{tr}(A_m^\top A_m)}{n} \right] \right\} \\ &= \operatorname{argmin}_{m \in \mathcal{M}} \{ \operatorname{crit}_C^{\text{lin}}(m) \} \\ \text{with } \operatorname{crit}_C^{\text{lin}}(m) &:= \frac{1}{n} \left( \|(I_n - A_m)F\|^2 + (C - \sigma^2) [2 \operatorname{tr}(A_m) - \operatorname{tr}(A_m^\top A_m)] \right), \end{aligned} \quad (49)$$

by Eq. (47). Let us assume that the approximation error term  $n^{-1} \|(I_n - A_m)F\|^2$ , which appears in Eq. (46), is a decreasing function of the degrees of freedom  $\mathcal{E}_m = \operatorname{tr}(A_m)$ ; let us also assume for simplicity that  $0 \leq \operatorname{tr}(A_m^\top A_m) \leq \operatorname{tr}(A_m)$  for every  $m \in \mathcal{M}$ . Then, we can distinguish two cases:

- if  $C < \sigma^2$ , then  $\operatorname{crit}_C^{\text{lin}}(m)$  is a decreasing function of  $\mathcal{E}_m$ , and  $\mathcal{E}_{m_{\min}^{\star \text{lin}}(C)}$  is huge:  $m_{\min}^{\star \text{lin}}(C)$  overfits.
- if  $C > \sigma^2$ , then  $\operatorname{crit}_C^{\text{lin}}(m)$  increases with  $\mathcal{E}_m$  for  $\mathcal{E}_m$  large enough, so  $\mathcal{E}_{m_{\min}^{\star \text{lin}}(C)}$  is much smaller than when  $C < \sigma^2$ .

This behavior is also the one of  $\widehat{m}_{\min}^{\text{lin}}(C)$ , as illustrated in Figure 3 (red curve / crosses), which leads to the following algorithm.

**Algorithm 4** (Minimal-penalty algorithm for linear estimators).

Input:  $(\|\widehat{F}_m - Y\|^2)_{m \in \mathcal{M}}$ ,  $(\operatorname{tr}(A_m))_{m \in \mathcal{M}}$ , and  $(\operatorname{tr}(A_m^\top A_m))_{m \in \mathcal{M}}$ .

1. Compute  $(\widehat{m}_{\min}^{\text{lin}}(C))_{C \geq 0}$ , where  $\widehat{m}_{\min}^{\text{lin}}(C)$  is defined by Eq. (49).
2. Find  $\widehat{C}_{\text{jump}} > 0$  corresponding to the “unique large jump” of  $C \mapsto \operatorname{tr}(A_{\widehat{m}_{\min}^{\text{lin}}(C)})$ .
3. Select  $\widehat{m}_{\text{Alg.4}} \in \operatorname{argmin}_{m \in \mathcal{M}} \{ n^{-1} \|\widehat{F}_m - Y\|^2 + 2\widehat{C}_{\text{jump}} \operatorname{tr}(A_m)/n \}$ .

Output:  $\widehat{m}_{\text{Alg.4}}$ .

Theorem 1 can be extended to Algorithm 4, up to some minor changes in the assumptions and results (Arlot and Bach, 2009, 2011). For kernel ridge regression, Algorithm 4 is proved to work also for choosing over a continuous set  $\mathcal{M}$  (Arlot and Bach, 2011), provided the kernel is fixed.

Note that when  $\operatorname{tr}(A_m^\top A_m) = \operatorname{tr}(A_m)$ ,  $\operatorname{pen}_{\text{opt}}(m) = 2 \operatorname{pen}_{\min}^{\text{lin}}(m)$ . This occurs for least-squares estimators —for which  $A_m = A_m^\top A_m = \Pi_m$ , and we recover the setting of Section 2 and Algorithm 1— and for  $k$ -nearest neighbors estimators.

### 3.5. General minimal-penalty algorithm

We now go back to the general setting of Section 3.1, and propose a generalization of Algorithms 1 and 4. Here, we suggest to take  $\widehat{C}_{\text{jump}} = \widehat{C}_{\text{window}}$ , but any other formal definition of  $\widehat{C}_{\text{jump}}$  could be used instead.

**Algorithm 5** (General minimal-penalty algorithm, jump formulation).

Input:  $(\widehat{\mathcal{R}}_n(\widehat{s}_m))_{m \in \mathcal{M}}$ ,  $(\operatorname{pen}_0(m))_{m \in \mathcal{M}}$ ,  $(\operatorname{pen}_1(m))_{m \in \mathcal{M}}$ ,  $(\mathcal{E}_m)_{m \in \mathcal{M}}$ , and  $\eta \geq 0$ .

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1. Compute  $(\widehat{m}_{\min}^{(0)}(C))_{C \geq 0}$ , where for every  $C \geq 0$ ,

$$\widehat{m}_{\min}^{(0)}(C) \in \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \widehat{\mathcal{R}}_n(\widehat{s}_m) + C \operatorname{pen}_0(m) \right\}. \quad (50)$$

2. Find  $\widehat{C}_{\text{jump}} > 0$  corresponding to the “unique large jump” of  $C \mapsto \mathcal{E}_{\widehat{m}_{\min}^{(0)}(C)}^{(0)}$ , for instance,

$$\widehat{C}_{\text{window}} \in \operatorname{argmax}_{C > 0} \left\{ \mathcal{E}_{\widehat{m}_{\min}^{(0)}(C/[1+\eta])}^{(0)} - \mathcal{E}_{\widehat{m}_{\min}^{(0)}(C[1+\eta])}^{(0)} \right\}.$$

3. Select  $\widehat{m}_{\text{Alg.5}} \in \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \widehat{\mathcal{R}}_n(\widehat{s}_m) + \widehat{C}_{\text{jump}} \operatorname{pen}_1(m) \right\}$ .

Output:  $\widehat{m}_{\text{Alg.5}}$ .

Algorithm 5 implicitly assumes that the minimal and the optimal penalty are respectively equal to  $C^* \operatorname{pen}_0$  and  $C^* \operatorname{pen}_1$ , with  $\operatorname{pen}_0$  and  $\operatorname{pen}_1$  known, but  $C^*$  unknown. We refer to Section 7.1 for practical remarks about the choice of  $\widehat{C}_{\text{jump}}$ . Computational issues are discussed in Section 7.2.

In the “slope heuristics” setting (Section 2),  $\operatorname{pen}_1 = 2 \operatorname{pen}_0$ , and Algorithm 5 reduces to Algorithm 3.

Similarly to Algorithm 2, we can also propose a “slope” formulation of Algorithm 5.

**Algorithm 6** (General minimal-penalty algorithm, slope formulation).

Input:  $(\widehat{\mathcal{R}}_n(\widehat{s}_m))_{m \in \mathcal{M}}$ ,  $(\operatorname{pen}_0(m))_{m \in \mathcal{M}}$ ,  $(\operatorname{pen}_1(m))_{m \in \mathcal{M}}$ , and  $(\mathcal{E}_m)_{m \in \mathcal{M}}$ .

1. Estimate the slope  $\widehat{C}_{\text{slope}}$  of  $-\widehat{\mathcal{R}}_n(\widehat{s}_m)$  as a function of  $\operatorname{pen}_0(m)$  for all  $m \in \mathcal{M}$  with  $\mathcal{E}_m$  “large enough”, for instance by (robust) linear regression.
2. Select  $\widehat{m}_{\text{Alg.6}} \in \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \widehat{\mathcal{R}}_n(\widehat{s}_m) + \widehat{C}_{\text{slope}} \operatorname{pen}_1(m) \right\}$ .

Output:  $\widehat{m}_{\text{Alg.6}}$ .

What remains now is to identify natural candidates for being a minimal or an optimal penalty in the general setting.

### 3.6. Optimal and minimal penalties

In the general setting, the unbiased risk estimation heuristics (Akaike, 1970; Stein, 1981) suggests the following optimal (deterministic) penalty

$$\operatorname{pen}_{\text{opt}}^{\text{gal}}(m) := \mathbb{E} \left[ \mathcal{R}(\widehat{s}_m) - \widehat{\mathcal{R}}_n(\widehat{s}_m) \right] \quad (51)$$

which generalizes formula (4). If  $\mathcal{R}(\widehat{s}_m) - \widehat{\mathcal{R}}_n(\widehat{s}_m)$  is concentrated around its expectation uniformly over  $m \in \mathcal{M}$  —which excludes too large collections  $\mathcal{M}$ —, one can prove an oracle inequality for the penalty (51), or for any penalty which differs from Eq. (51) by an additive term independent from  $m$ , as in Eq. (9) and (48).

Building a minimal penalty in the general setting is more difficult. For every  $m \in \mathcal{M}$ , let  $\mathcal{E}_m$  be some “complexity measure” associated with  $\widehat{s}_m$ , that is, we assume that the empirical risk  $\widehat{\mathcal{R}}_n(\widehat{s}_m)$

(or its expectation) is (approximately) a decreasing function of  $\mathcal{C}_m$ . Algorithm 6 suggests that the minimal penalty is a quantity which exactly compensates this decreasing trend, such as

$$\text{pen}_{\min,0}^{\text{gal}}(m) := -\mathbb{E}[\widehat{\mathcal{R}}_n(\widehat{s}_m)]. \quad (52)$$

Nevertheless, in most cases including least-squares and linear estimators,  $\text{pen}_{\min,0}^{\text{gal}}$  is unknown, even up to a multiplicative factor, so that we need another candidate for being a minimal penalty.

For every  $m \in \mathcal{M}$ , let  $s_m^*$  be a well-chosen element of  $\mathbb{S}$  —see Remark 2 below— such that  $\mathcal{R}(s_m^*) - \inf_{t \in \mathbb{S}} \mathcal{R}(t)$  decreases to zero as  $\mathcal{C}_m \rightarrow \infty$ . As argued below, a natural choice for the minimal penalty is

$$\text{pen}_{\min}^{\text{gal}}(m) := \mathbb{E}[\widehat{\mathcal{R}}_n(s_m^*) - \widehat{\mathcal{R}}_n(\widehat{s}_m)]. \quad (53)$$

Indeed, for every  $C \geq 0$  let

$$\text{crit}_C^{\text{gal}}(m) := \mathbb{E}[\widehat{\mathcal{R}}_n(\widehat{s}_m)] + C \text{pen}_{\min}^{\text{gal}}(m) = C \mathcal{R}(s_m^*) + (1-C) \mathbb{E}[\widehat{\mathcal{R}}_n(\widehat{s}_m)] \quad (54)$$

so that  $m_{\min}^{\text{gal}^*}(C) \in \text{argmin}_{m \in \mathcal{M}} \{\text{crit}_C^{\text{gal}}(m)\}$  is a proxy for

$$\widehat{m}_{\min}^{\text{gal}}(C) \in \text{argmin}_{m \in \mathcal{M}} \{\widehat{\mathcal{R}}_n(\widehat{s}_m) + C \text{pen}_{\min}^{\text{gal}}(m)\}.$$

Let us assume for simplicity that  $\widehat{\mathcal{R}}_n(\widehat{s}_m)$  is a decreasing function of  $\mathcal{C}_m$ . Then, when  $C < 1$ ,  $\text{crit}_C^{\text{gal}}(m)$  is a decreasing function of  $\mathcal{C}_m$ , so that  $\mathcal{C}_{m_{\min}^{\text{gal}^*}(C)} \approx \max_{m \in \mathcal{M}} \mathcal{C}_m$  which corresponds to overfitting. On the contrary, when  $C > 1$ ,  $(1-C) \mathbb{E}[\widehat{\mathcal{R}}_n(\widehat{s}_m)]$  is an increasing function of  $\mathcal{C}_m$  while  $C \mathcal{R}(s_m^*)$  is approximately constant for  $\mathcal{C}_m$  large enough, so that  $\mathcal{C}_{m_{\min}^{\text{gal}^*}(C)} \ll \max_{m \in \mathcal{M}} \mathcal{C}_m$ . Therefore, if concentration inequalities show that  $\widehat{m}_{\min}^{\text{gal}}(C)$  behaves like  $m_{\min}^{\text{gal}^*}(C)$ ,  $\text{pen}_{\min}^{\text{gal}}$  is a minimal penalty.

Let us emphasize that for making use of the fact that  $\text{pen}_{\min}^{\text{gal}}$  is a minimal penalty, we must assume that  $\text{pen}_{\min}^{\text{gal}} \approx C^* \text{pen}_0$  and  $\text{pen}_{\text{opt}}^{\text{gal}} \approx C^* \text{pen}_1$  for some unknown  $C^* > 0$  and some *known* penalty shapes  $\text{pen}_0$  and  $\text{pen}_1$ . Remark that we could generalize this assumption to the existence of some known function  $f$  such that  $\text{pen}_{\min}^{\text{gal}} \approx C^* \text{pen}_0$  and  $\text{pen}_{\text{opt}}^{\text{gal}} \approx f(C^*) \text{pen}_1$ , but such a generalization has not been proved useful yet.

**Remark 2** (Choice of  $s_m^*$ ). *Overall, the above heuristics makes two assumptions on  $s_m^* \in \mathbb{S}$ . First,  $\mathcal{R}(s_m^*) - \inf_{t \in \mathbb{S}} \mathcal{R}(t)$  is small when  $\mathcal{C}_m$  is large. Second,  $\text{pen}_{\min}^{\text{gal}}(m)$  is known up to a multiplicative constant, whose value can be used for deriving an optimal penalty. When  $\widehat{s}_m \in \text{argmin}_{t \in \mathbb{S}_m} \widehat{\mathcal{R}}_n(t)$  is an empirical risk minimizer over some model  $\mathbb{S}_m \subset \mathbb{S}$ , a natural choice is  $s_m^* \in \text{argmin}_{t \in \mathbb{S}_m} \mathcal{R}(t)$ , so that  $\mathcal{R}(s_m^*) - \inf_{t \in \mathbb{S}} \mathcal{R}(t)$  is the approximation error. For linear estimators, the decomposition (46) of the risk suggests to take  $s_m^* = A_m F$ . By analogy, we call  $\mathcal{R}(s_m^*) - \inf_{t \in \mathbb{S}} \mathcal{R}(t)$  the approximation error associated with  $\widehat{s}_m$  in the general case. Choosing  $s_m^*$  might be difficult in general; when this makes sense, an option is the expectation of  $\widehat{s}_m$ .*

### 3.7. Bibliographical remarks

**Algorithms** The slope-heuristics algorithm for calibrating penalties was first proposed in the Gaussian least-squares regression setting of Section 2 with a penalty proportional to the dimension (Birgé and Massart, 2001b), as in Algorithms 1–2. Then, it was generalized to a penalty

function of the dimension (Birgé and Massart, 2007), and to a general penalty shape (Massart, 2005; Blanchard and Massart, 2006; Massart, 2007), as in Algorithm 3.

The first implementations of the slope heuristics were done directly with Algorithm 3 (or its “slope” version) with  $\mathcal{C}_m = D_m$ , instead of Algorithms 1–2, since they were outside the setting of Section 2: maximum-likelihood estimators (Letu e, 2000, Section A.4), and change-point detection (Lebarbier, 2002, Chapter 4).

The proposition of using a general complexity measure  $\mathcal{C}_m$  instead of a dimension  $D_m$  (as in Algorithms 3, 5–6) was first made in density estimation (Lerasle, 2009), with the suggestion of estimating  $\mathcal{C}_m$  by resampling if necessary.

The failure of Algorithm 3 for linear estimators in regression was noticed by Arlot and Bach (2009), where Algorithm 4 was proposed and theoretically justified. The general Algorithm 5 has only been formalized by Arlot (2011, Section 2.5), while its “slope estimation” version (Algorithm 6) is new, even if the (approximate) equivalence between “jump” and “slope” algorithms is not. Up to now, the general formulation of Algorithms 5–6 has only been proved useful in the case of linear estimators in regression (Arlot and Bach, 2009, 2011) and in density estimation (Magalh aes, 2015; Lerasle et al., 2016), with different shapes for  $\text{pen}_0$  and  $\text{pen}_1$ . It can also be useful in a few other settings where  $\text{pen}_1$  is proportional to  $\text{pen}_0$  but the ratio between optimal and minimal penalty might be different from 2, for selecting among a rich collection of models or estimators. For instance, for pruning a decision tree, the “max” variant considered by Bar-Hen et al. (2018, Section 5.4) is equivalent to Algorithm 5 with  $\text{pen}_1 = \text{pen}_0$ , hence selecting the estimator “just after” the maximal jump.

**Theory** The first (partial) theoretical result proved outside the setting of Section 2 was for maximum-likelihood estimators (histograms) in density estimation, assuming that the true density  $s^*$  is the uniform density over  $[0, 1]$  (Castellan, 1999). Other theoretical results outside the setting of Section 2 are reviewed in Section 4.

The first theoretical result proved for Algorithm 3 with a penalty shape  $\text{pen}_1(m)$  *not* function of a dimension  $D_m$  was obtained in heteroscedastic least-squares regression (Arlot and Massart, 2009), where the penalty shape can be estimated by resampling (Arlot, 2009).

The general heuristics “ $\text{pen}_{\text{opt}} \approx 2\text{pen}_{\text{min}}$ ” underlying Algorithm 3 was formulated by Blanchard and Massart (2006, Section 2) and Massart (2007, Section 8.5.2), together with a heuristic argument for suggesting

$$p_2(m) := \widehat{\mathcal{R}}_n(s_m^*) - \widehat{\mathcal{R}}_n(\widehat{s}_m)$$

as a minimal penalty, when  $\widehat{s}_m$  is an empirical risk minimizer and  $s_m^*$  is defined according to Remark 2. In these papers,  $p_2(m)$  is called  $\widehat{v}_m$  since it can be interpreted as a variance. Here, the general minimal penalty that we propose is  $\text{pen}_{\text{min}}^{\text{gal}}(m) = \mathbb{E}[p_2(m)]$ , as in the PhD dissertation of Arlot (2007, Chapter 3) for instance. Another formulation of the heuristics behind Algorithm 3 is “ $p_1(m) \approx p_2(m)$ ”, where

$$p_1(m) := \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s_m^*),$$

as for instance written in a binary classification framework by Zwald (2005, Section 6.4.3), together with “ $p_2(m) \propto D_m$  for  $D_m$  large enough”.

#### 4. Theoretical results: a review

This section collects all theoretical results that are directly related to minimal-penalty algorithms, to the best of our knowledge. First, the proof of Algorithm 5 is split into several subproblems (Section 4.1). Then, we present full proofs of Algorithm 5 (Section 4.2) and partial results (Sections 4.3–4.7). Note that some related results outside the setting of Section 3 are reported in conclusion (Sections 8.3.6 and 8.5).

In this section, all partial or full proofs of Algorithm 5 that we present define  $\widehat{C}_{\text{jump}}$  as  $\widehat{C}_{\text{thr.}}(T_n)$  or  $\widehat{C}_{\text{window}}(\eta)$  for some well-chosen  $T_n$  or  $\eta$ . For the sake of simplicity, we do not discuss anymore the exact definition chosen for  $\widehat{C}_{\text{jump}}$ , until we tackle this question in Section 7.1.

##### 4.1. General approach for proving Algorithm 5

Following Theorem 1 and its proof, let us suggest a general approach towards a theoretical justification of Algorithm 5, that we split into several subproblems.

- ( $\alpha$ ) **The minimal and optimal penalties are known up to some common multiplicative factor:** Find two penalty functions  $\text{pen}_0$ ,  $\text{pen}_1$ , and a complexity measure  $(\mathcal{C}_m)_{m \in \mathcal{M}}$ , such that for some (unknown)  $C^* > 0$ ,  $C^* \text{pen}_0$  is a minimal penalty and  $C^* \text{pen}_1$  is an optimal penalty.
- ( $\beta$ )  $C^* \text{pen}_0$  **is actually a minimal penalty:**  $\eta_n^-, \eta_n^+ > 0$  exist such that, on a large-probability event,

$$\forall C < (1 - \eta_n^-) C^*, \quad \mathcal{C}_{\widehat{m}_{\min}^{(0)}(C)} \geq \mathcal{C}_{\text{overfit}} \propto \max_{m \in \mathcal{M}} \mathcal{C}_m \quad (\beta^-)$$

$$\forall C > (1 + \eta_n^+) C^*, \quad \mathcal{C}_{\widehat{m}_{\min}^{(0)}(C)} \leq \mathcal{C}_{\text{small}} \ll \max_{m \in \mathcal{M}} \mathcal{C}_m \quad (\beta^+)$$

$$\text{where} \quad \forall C \geq 0, \quad \widehat{m}_{\min}^{(0)}(C) \in \underset{m \in \mathcal{M}}{\text{argmin}} \left\{ \widehat{\mathcal{R}}_n(\widehat{s}_m) + C \text{pen}_0(m) \right\}.$$

The above statements about  $\mathcal{C}_{\widehat{m}_{\min}^{(0)}(C)}$  are vague on purpose, since the range of  $(\mathcal{C}_m)_{m \in \mathcal{M}}$  is not specified. When  $\mathcal{C}_m$  is the dimension  $D_m \in [1, n]$  of some model, one can specify  $\mathcal{C}_{\text{overfit}}$  and  $\mathcal{C}_{\text{small}}$  similarly to Eq. (14) and (16), respectively.

- ( $\gamma$ )  $C^* \text{pen}_1$  **is actually an optimal penalty:** there exists  $\eta > 0$  such that, on a large-probability event, for every  $C \in ([1 - \eta]C^*, [1 + \eta]C^*)$ ,

$$\begin{aligned} \forall \widehat{m}_{\text{opt}}^{(1)}(C) \in \underset{m \in \mathcal{M}}{\text{argmin}} \left\{ \widehat{\mathcal{R}}_n(\widehat{s}_m) + C \text{pen}_1(m) \right\}, \\ \mathcal{R}(\widehat{s}_{\widehat{m}_{\text{opt}}^{(1)}(C)}) - \mathcal{R}(s^*) \leq (1 + \varepsilon_n(\eta)) \inf_{m \in \mathcal{M}} \left\{ \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*) \right\} + R_n(\eta) \end{aligned} \quad (\gamma)$$

where  $\lim_{\eta \rightarrow 0, n \rightarrow +\infty} \varepsilon_n(\eta) = 0$  and the remainder term  $R_n(\eta)$  is negligible in front of the oracle risk  $\inf_{m \in \mathcal{M}} \left\{ \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*) \right\}$ .

As in the PhD dissertation of Arlot (2007), we use in this section the following notation:

$$p_1(m) := \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s_m^*), \quad (55)$$

$$p_2(m) := \widehat{\mathcal{R}}_n(s_m^*) - \widehat{\mathcal{R}}_n(\widehat{s}_m), \quad (56)$$

$$\text{and} \quad \delta(m) := \mathcal{R}(s_m^*) - \widehat{\mathcal{R}}_n(s_m^*). \quad (57)$$

In particular, with the notation of Section 3.6,

$$\text{pen}_{\text{opt}}^{\text{gal}}(m) = \mathbb{E}[p_1(m) + \delta(m) + p_2(m)] \quad \text{and} \quad \text{pen}_{\text{min}}^{\text{gal}}(m) = \mathbb{E}[p_2(m)].$$

#### 4.2. Full proofs of Algorithm 5

Few settings exist where a full proof of Algorithm 5 is available, that is, a proof that  $(\beta^-)$ ,  $(\beta^+)$ , and  $(\gamma)$  hold true on a large-probability event for some known  $\text{pen}_0$ ,  $\text{pen}_1$ ,  $(\mathcal{C}_m)_{m \in \mathcal{M}}$  and some (unknown)  $C^*$ . In this article,  $\mathcal{M}$  is always assumed to be finite with  $\text{card}(\mathcal{M}) \leq L_1 n^{L_2}$  for some  $L_1, L_2 > 0$ , except in Section 4.7.

We first collect results assuming that  $\text{pen}_1 = 2\text{pen}_0$ , so that Algorithm 5 reduces to Algorithm 3. Without explicit mention of the contrary, for all results reviewed in the list below, the noise is assumed independent and identically distributed,  $\hat{s}_m \in \text{argmin}_{t \in S_m} \hat{\mathcal{R}}_n(t)$  is an empirical risk minimizer, so we take  $s_m^* \in \text{argmin}_{t \in S_m} \mathcal{R}(t)$  for defining  $p_2(m)$ , and the complexity used is  $\mathcal{C}_m = D_m$  the dimension of  $S_m$ . Full proofs of Algorithm 5 exist in the following settings:

- *Regression on a fixed design, homoscedastic (sub-)Gaussian noise, least-squares risk and estimators:* Birgé and Massart (2007) and Theorem 1 (and Remark 1 for the sub-Gaussian case) prove it with  $\text{pen}_0(m) = D_m/n$  and  $C^* = \sigma^2$  the (constant) noise level. Note that  $p_1(m) = p_2(m) = n^{-1} \|\Pi_m \varepsilon\|^2$  in this setting.
- *Regression on a random design, heteroscedastic noise* (not necessarily Gaussian), least-squares risk, with various least-squares estimators: regressograms with moment assumptions on the noise (Arlot and Massart, 2009), piecewise polynomials with bounded noise (Saumard, 2013, with key concentration results for  $p_1$  and  $p_2$  proved by Saumard, 2012), or more general models satisfying a “strongly-localized basis” assumption with bounded noise (Saumard, 2010a; Navarro and Saumard, 2017). Contrary to the previous setting,  $\mathbb{E}[p_1(m)] \approx \mathbb{E}[p_2(m)]$  holds true only for most models and for  $n$  large enough. The penalty shape  $\text{pen}_0(m) = \mathbb{E}[p_2(m)]$  is unknown in general and  $C^* = 1$ . For regressograms, the results remain true when  $\text{pen}_0(m)$  is a resampling-based estimation of  $\mathbb{E}[p_2(m)]$  (see Arlot, 2009). For piecewise polynomials, the same holds when  $\text{pen}_0(m)$  is a hold-out estimation of  $\mathbb{E}[p_2(m)]$  (see Saumard, 2013). For strongly localized bases, the (approximate) closed-form formula for  $\mathbb{E}[p_1(m)]$  and  $\mathbb{E}[p_2(m)]$  provided by Navarro and Saumard (2017, Theorem 6.3) might be used for estimating  $\text{pen}_0(m)$  without resampling; another option is  $V$ -fold penalization (Navarro and Saumard, 2017, Section 5).
- *Density estimation, least-squares risk and estimators, i.i.d.* (Lerasle, 2012) or *mixing data* (Lerasle, 2011). The penalty shape  $\text{pen}_0(m) = \mathbb{E}[p_2(m)]$  is approximately known for some specific models (regular histograms), in general it can be estimated by resampling as previously. In this setting, the complexity  $\mathcal{C}_m$  can either be the dimension of  $S_m$  or the resampling-based estimator of  $\mathbb{E}[p_2(m)]$  itself. Note that in least-squares density estimation, we have  $p_1(m) = p_2(m)$  almost surely.
- *Density estimation, Kullback risk and maximum-likelihood estimators, histogram models* (Saumard, 2010c). This result is the first one obtained without the least-squares risk. The penalty shape  $\text{pen}_0(m) = D_m/(2n)$  is known,  $C^* = 1$ , and the optimal penalty is AIC. A partial result, for the uniform density over  $[0, 1]$  only, has previously been proved by Castellan (1999).

- *Specification probabilities in general random fields* (that is, graphical models), least-squares or Kullback risks, estimators that are empirical distributions conditionally to the values observed on a subset  $m$  of the field (Lerasle and Takahashi, 2016). The shape of the penalty and the complexity  $\text{pen}_0(m) = \mathcal{C}_m = p_2(m)$  are unknown. The authors suggest to use instead the shape of a theoretical upper bound on  $\mathbb{E}[p_2(m)]$ , dropping off pessimistic constants, with convincing experimental results.

The above results for least-squares regression on a random design, least-squares density estimation (i.i.d. case), and maximum-likelihood density estimation can all be recovered (sometimes up to minor differences) as a corollary of a general result which holds for all “regular estimators” (Saumard, 2010b, Chapters 7–8).

Full proofs of Algorithm 5 (or a slight modification of it) also exist in two settings where  $\text{pen}_1 \neq 2\text{pen}_0$  in general:

- Regression on a fixed design, independent and identically distributed (homoscedastic) Gaussian noise, least-squares risk, *linear estimators*: Arlot and Bach (2009, 2011) prove that Algorithm 4 works, while Algorithm 3 fails in general, as detailed in Sections 3.2–3.3.
- Density estimation, independent and identically distributed data, least-squares risk, *linear estimators* (for instance, Parzen density estimators and weighted least-squares estimators): Lerasle et al. (2016) —after a preliminary version in the PhD dissertation of Magalhães (2015, Chapter 2)— define some theoretical quantities  $\text{pen}_0(m) \approx \mathbb{E}[p_2(m)]$  and  $\mathcal{C}_m \approx \mathbb{E}[p_1(m)]$  —easy to estimate in general, and known for several examples such as Parzen density estimators— such that

$$\hat{m}(C) \in \underset{m \in \mathcal{M}}{\text{argmin}} \left\{ \widehat{\mathcal{R}}_n(\hat{s}_m) + \text{pen}_0(m) + C\mathcal{C}_m \right\}$$

overfits for  $C < 0$  and satisfies an oracle inequality for all  $C > 0$ , first-order optimal when  $C = C^* = 1$ . In other words, Lerasle et al. (2016) almost prove that Algorithm 5 works with  $\text{pen}_0(m) = \mathbb{E}[p_2(m)]$ ,  $\text{pen}_1(m) = \mathbb{E}[p_1(m)] + \mathbb{E}[p_2(m)]$ ,  $\mathcal{C}_m = \mathbb{E}[p_1(m)]$ , and  $C^* = 1$ . This result implies the one of Lerasle (2012) for least-squares estimators. A noticeable fact in this framework is that  $\text{pen}_{\min}$  —and sometimes even  $\text{pen}_{\text{opt}}$ , surprisingly— can be negative, making the terminology “minimal” penalty questionable (Lerasle et al., 2016, Sections 4.3 and 5). Note that  $\text{pen}_{\text{opt}}$  here can be negative because  $\hat{s}_m$  is not an empirical risk minimizer, hence  $\widehat{\mathcal{R}}_n(\hat{s}_m)$  is not necessarily biased downwards as an estimator of  $\mathcal{R}(\hat{s}_m)$ . Nevertheless, for most usual estimators,  $\text{pen}_{\min}$  and  $\text{pen}_{\text{opt}}$  are always positive. Theoretical results for choosing among Parzen density estimators with slightly different minimal-penalty algorithms —closer to Goldenshluger-Lepski’s method— are discussed in Section 8.5.

**Remark 3** (Minimal penalties with resampling-based estimators of  $\mathbb{E}[p_2(m)]$ ). *In several papers mentioned above, theoretical results validate Algorithm 5 with  $\text{pen}_0(m) = \mathcal{C}_m = p_2(m)$  or  $\mathbb{E}[p_2(m)]$ ,  $\text{pen}_1(m) = 2\text{pen}_0(m)$ , and  $C^* = 1$ . Such results might seem useless since (i)  $\text{pen}_0$  is unknown, and (ii)  $C^*$  is known, that is, the exact opposite of the motivation for Algorithm 5 exposed in Section 3.2. Nevertheless, problem (i) can be solved by taking  $\text{pen}_0(m) = \mathcal{C}_m$  equal to a resampling-based estimator  $\hat{p}_2^W(m)$  of  $\mathbb{E}[p_2(m)]$  (Lerasle, 2012, for instance). Then, as usual*



with resampling, it remains to find the constant  $C_W$  such that  $C_W \mathbb{E}[\widehat{p}_2^W(m)] \approx \mathbb{E}[p_2(m)]$  for all  $m \in \mathcal{M}$ . When such a constant  $C_W$  exists, it usually depends on the resampling scheme  $W$ , the sample size, and the particular setting considered (Arlot, 2009). As a consequence, we recover a setting where  $\text{pen}_0(m) = \mathcal{C}_m = \widehat{p}_2^W(m)$  is known and  $C^* = C_W$  is unknown, for which Algorithm 5 can be useful. Note that we here propose to take  $\mathcal{C}_m = \widehat{p}_2^W(m)$ , which does not estimate  $\mathbb{E}[p_2(m)]$  but  $\mathbb{E}[p_2(m)]/C_W$ ; this is not a problem since the complexity jump is independent from the rescaling by  $C_W$ .

According to simulation experiments, the above strategy of combining resampling penalties with the slope heuristics can be better (Lerasle, 2010, least-squares density estimation) or worse (Garivier and Lerasle, 2011, context-tree estimation) compared to using the penalty  $\widetilde{C}_W \widehat{p}_2^W(m)$ , where  $\widetilde{C}_W$  derives from asymptotic theoretical results and does not depend on any unknown quantity in the settings of these two articles.

### 4.3. Partial proofs: uncertainty on the optimal penalty

An optimal oracle inequality like  $(\gamma)$  in Section 4.1 has not been proved in many frameworks, and it is quite difficult to obtain a leading constant  $1 + \varepsilon_n(\eta) = 1 + o(1)$  while keeping the remainder term negligible in front of the oracle risk. A much more usual result in the model-selection literature is the following weakened version of  $(\gamma)$ : on a large-probability event, for every  $C \in ([1 - \eta]C^*, [1 + \eta]C^*)$  with  $\eta > 0$  small enough,

$$\mathcal{R}\left(\widehat{s}_{\widehat{m}_{\text{opt}}(C)}^{(1)}\right) - \mathcal{R}(s^*) \leq K_n(\eta) \inf_{m \in \mathcal{M}} \left\{ \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*) \right\} + R_n(\eta) \quad (\widetilde{\gamma})$$

for some  $K_n(\eta), R_n(\eta) < \infty$ . Note that  $(\gamma)$  with  $\varepsilon_n = 0$  and  $R_n \geq \inf_{m \in \mathcal{M}} \left\{ \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*) \right\}$  should be understood as  $(\widetilde{\gamma})$  with  $K_n \geq 2$ . Similarly, a classical way to write an oracle-type inequality is

$$\mathcal{R}\left(\widehat{s}_{\widehat{m}_{\text{opt}}(C)}^{(1)}\right) - \mathcal{R}(s^*) \leq \inf_{m \in \mathcal{M}} \left\{ \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*) + R_n(m) \right\}. \quad (\widetilde{\gamma}')$$

When  $R_n(m)$  is comparable to  $\mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*)$ , or even larger, (for instance,  $R_n(m) \geq \text{pen}(m)$ ),  $(\widetilde{\gamma}')$  should be understood as  $(\widetilde{\gamma})$  with  $K_n \geq 2$ .

Proving only  $(\widetilde{\gamma})$  instead of  $(\gamma)$  is a significant limitation:  $(\widetilde{\gamma})$  does not show that  $C^* \text{pen}_1$  is an optimal penalty if we cannot prove that  $K_n(\eta)$  is first-order optimal, which is very difficult to prove unless  $K_n(\eta) = 1 + o(1)$  as in  $(\gamma)$ . As a consequence, in such cases,  $C^* \text{pen}_1$  might not be optimal, and the optimal penalty might be  $C' \text{pen}_1$  with  $C^* \neq C'$ , or even have a completely different shape than  $\text{pen}_1$ . For instance, in the setting of Section 3.4, the optimal penalty is  $2\sigma^2 \text{tr}(A_m)/n$ , but taking  $2\sigma^2[\text{tr}(A_m) + \text{tr}(A_m^\top A_m)]/n$  as a penalty, we could have an oracle inequality  $(\widetilde{\gamma})$  with a penalty having a suboptimal shape.

**Results** Nevertheless, proving  $(\beta)$  and  $(\widetilde{\gamma})$  still shows that Algorithm 5 provides a data-driven estimator satisfying an oracle inequality. Such a result exists for context-tree estimation with the Kullback risk,  $\phi$ -mixing processes, and maximum-likelihood estimators (Garivier and Lerasle, 2011), with  $\text{pen}_0(m) = \mathcal{C}_m = p_2(m)$  and  $\text{pen}_1(m) = 2 \text{pen}_0(m)$ . Simulation experiments suggest that  $p_2(m)$  can be replaced by a BIC-type penalty or a resampling-based estimator of  $\mathbb{E}[p_2(m)]$ ,

see Remark 3 in Section 4.2. What is missing to get a proof of  $(\gamma)$  is a tight concentration inequality for  $\delta(m) - \delta(m')$ , that is, to have Eq. (60) satisfied with  $\varepsilon_\delta = o(1)$  as required in Proposition 2, see Section 5.2.2. Simulation experiments suggest that  $\text{pen}_1 = 2\text{pen}_0$  is indeed an optimal choice here.

#### 4.4. Minimal penalty in terms of risk: $(\beta')$

Another way to define a minimal penalty is in terms of the risk of  $\widehat{s}_{\widehat{m}_{\min}^{(0)}(C)}$ , which is theoretically interesting but does not prove the presence of a complexity jump as expected by Algorithm 5:

$$\forall C < (1 - \eta_n^-)C^*, \mathcal{R}\left(\widehat{s}_{\widehat{m}_{\min}^{(0)}(C)}\right) - \mathcal{R}(s^*) \geq \kappa \max_{m \in \mathcal{M}} \{\mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*)\} \quad (\beta'^-)$$

$$\forall C > (1 + \eta_n^+)C^*, \mathcal{R}\left(\widehat{s}_{\widehat{m}_{\min}^{(0)}(C)}\right) - \mathcal{R}(s^*) \leq K \left(\frac{C}{C^*}\right) \inf_{m \in \mathcal{M}} \{\mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*)\} + R_n \left(\frac{C}{C^*}\right) \quad (\beta'^+)$$

where for every  $x > 1$ ,  $K(x) \in [1, \infty)$  and  $R_n(x) \ll \inf_{m \in \mathcal{M}} \{\mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*)\}$  in general, and  $\kappa > 0$  is an absolute constant.

When  $(\beta)$ , which is defined in Section 4.1, is replaced by  $(\beta')$  above, the justification of Algorithm 5 is far from being complete, since there might be no complexity jump as required in the definition of  $\widehat{C}_{\text{window}}$ . Nevertheless, once  $(\beta')$  is proved, one can reasonably conjecture that  $(\beta)$  holds true under similar assumptions, provided that  $\mathcal{C}_m$  is well chosen. Moreover,  $(\beta)$  and  $(\beta')$  are closely related if

$$\forall x > 0, \quad \inf_{m \in \mathcal{M} / \mathcal{C}_m \geq x} \{\mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*)\} \geq g(x) > 0 \quad (58)$$

for some increasing function  $g$ . Indeed, assuming (58),  $(\beta^-)$  implies  $(\beta'^-)$  with

$$\kappa = \frac{g(\mathcal{C}_{\text{overfit}})}{\max_{m \in \mathcal{M}} \{\mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*)\}},$$

and  $(\beta'^+)$  implies  $(\beta^+)$  with

$$\mathcal{C}_{\text{small}} = g^{-1} \left( K \left( \frac{C}{C^*} \right) \inf_{m \in \mathcal{M}} \{\mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*)\} \right) + R_n \left( \frac{C}{C^*} \right).$$

Note that Eq. (58) holds true with  $g(x) = x/\alpha$  if  $\mathcal{C}_m \approx \alpha p_1(m)$ ; for instance, for least-squares estimators and risk,  $\alpha = \sigma^2/n$  since  $\mathcal{C}_m = D_m$  and  $p_1(m) \approx \sigma^2 D_m/n$ . Let us remark finally that the proof of  $(\beta'^-)$  usually relies on a proof of  $(\beta^-)$ , sometimes hidden by technical details.

**Results** To the best of our knowledge, a full proof of  $(\beta')$  currently exists only in settings where  $(\beta)$  is proved to hold, except one result that we report in Section 4.7. Some partial proofs of  $(\beta')$  are reviewed in the next subsections.



#### 4.5. Partial proofs: uncertainty on the minimal penalty

A result weaker than  $(\beta)$  can be proved about the complexity jump: for some  $C_1^* < C_2^*$  (that remain distinct even when  $n \rightarrow +\infty$ ),

$$\forall C < C_1^*, \quad (\beta^-) \text{ holds true,} \quad \text{and} \quad \forall C > C_2^*, \quad (\beta^+) \text{ holds true.} \quad (\tilde{\beta})$$

In other words,  $C_1^* \text{pen}_0$  is a too small penalty, while  $C_2^* \text{pen}_0$  is a sufficiently large penalty.

From the theoretical point of view, proving  $(\tilde{\beta})$  instead of  $(\beta)$  is a serious limitation: for reasons similar to the ones explained in Section 4.3 for  $(\tilde{\gamma})$ , it can happen that  $\text{pen}_0$  is not the shape of a minimal penalty. For instance, in the setting of Section 3.3,  $(\tilde{\beta})$  holds true with  $\text{pen}_0(m) = \text{tr}(A_m)$  although this quantity is not always proportional to the minimal penalty, as shown by Figure 3.

Nevertheless, from the practical point of view, one can still derive from  $(\tilde{\beta})$  a way to get from data some  $\hat{C} \in [C_1^*, C_2^*]$ , for instance by taking a large  $\eta$  in the definition of  $\hat{C}_{\text{window}}(\eta)$ . If  $(C_2^*/C_1^*)$  is not too large and if  $(\tilde{\gamma})$  holds true for some  $C^* \in [C_1^*, C_2^*]$ , this leads to an estimator satisfying an oracle inequality.

**Results** One full proof of  $(\tilde{\beta})$  and  $(\tilde{\gamma})$  is available for prediction in a Gaussian graphical model via neighborhood selection, with conditional least-squares risk and estimators, a minimal-penalty shape  $\text{pen}_0(m) = \mathcal{C}_m = D_m$ , and an optimal penalty shape  $\text{pen}_1$  proportional to  $\text{pen}_0$  (Verzelen, 2010). The proof of  $(\tilde{\beta})$  assumes in addition that the graph is a square lattice. Simulation experiments suggest that there is indeed a jump around  $C^*$  and that Algorithm 5 works well.

#### 4.6. Partial proofs: for some specific $s^*$ only

The weakest partial proofs of  $(\beta)$  are the ones only valid for some particular  $s^*$ , which often is  $s^* = 0$ . Then, although  $C^* \text{pen}_0$  is a minimal penalty for this particular  $s^*$ , the general shape of the minimal penalty can differ from  $\text{pen}_0$ . For instance, in the Lasso case, an empirical study shows that the shape of  $\mathbb{E}[p_2(m)]$  depends on  $s^*$  and on some other features of the distribution of the data (Connault, 2011).

Nevertheless, such weak results still are a good way to guess  $\text{pen}_0$  for a practical use of Algorithm 5, and they can be a first step towards a full theoretical justification.

**Results** Such partial proofs exist in the case of multiplicative penalties, an apparently different setting that can still be cast into the framework of Algorithm 5. The principle, as exposed by Baraud et al. (2009) for least-squares regression, is to replace the penalized criterion (3) by the product of the empirical risk by some penalty term, that is, choosing

$$\hat{m} \in \underset{m \in \mathcal{M}}{\text{argmin}} \left\{ \hat{\mathcal{R}}_n(\hat{s}_m) \left( 1 + \frac{\text{pen}^{\text{mult}}(m)}{n - D_m} \right) \right\}. \quad (59)$$

This can actually be seen as an additive penalization method as in Eq. (3), with the penalty

$$\text{pen}(m) := \widehat{\mathcal{R}}_n(\widehat{s}_m) \frac{\text{pen}^{\text{mult}}(m)}{n - D_m}.$$

So, choosing a multiplicative factor in front of  $\text{pen}^{\text{mult}}(m)$  is equivalent to choosing a multiplicative factor in front of an additive penalty of a particular form. For fixed-design regression with least-squares risk and estimators, Baraud et al. (2009) prove that  $(\beta^-)$  holds true if  $s^* = 0$ , while  $(\beta'^+)$  and  $(\widetilde{\gamma})$  hold true in general, with  $C^* \text{pen}_0^{\text{mult}}(m) = D_m$  and  $\text{pen}_1^{\text{mult}} \propto \text{pen}_0^{\text{mult}}$ .

In addition, in the setting of multivariate regression on a fixed design with the least-squares risk and low-rank least-squares estimators,  $(\widetilde{\gamma})$  and  $(\beta'^+)$  are proved in a general case, while  $(\beta^-)$  is proved only for  $s^* = 0$  (Giraud, 2011); remark that  $(\beta^+)$  can certainly be proved in a general case, although its proof is not written in the article by Giraud (2011). Note also that these results are valid both for additive penalties and for multiplicative penalties as the ones of Baraud et al. (2009).

#### 4.7. Partial proofs: richer collections of models

Throughout the article, we assume (at least implicitly) that  $\mathcal{M}$  is not too large, that is,  $\text{card}(\mathcal{M})$  grows at most polynomially with the sample size  $n$ , or  $\mathcal{M}$  can be well approximated by such a polynomial set of estimators —e.g., kernel ridge regression with one continuous parameter  $\lambda$  (Arlot and Bach, 2011). Nevertheless, the case where  $\mathcal{M}$  is larger deserves attention, and we review in this subsection the partial results about minimal penalties in such settings. Note that each of them suffers from some of the limitations emphasized in Sections 4.3–4.6.

Let us consider the fixed-design regression setting, with least-squares risk and estimators on finite-dimensional vector spaces  $S_m$ . Assuming as Birgé and Massart (2007) that the penalty is a function of the dimension, the selected estimator

$$\widehat{s}_{\widehat{m}} \quad \text{with} \quad \widehat{m} \in \underset{m \in \mathcal{M}}{\text{argmin}} \{ \widehat{\mathcal{R}}_n(\widehat{s}_m) + \text{pen}(D_m) \}$$

can be rewritten as  $\widehat{s}'_D$  where

$$\forall D \in \mathbb{N}, \quad \widehat{s}'_D \in \underset{t \in S'_D}{\text{argmin}} \{ \widehat{\mathcal{R}}_n(t) \}, \quad S'_D := \bigcup_{\substack{m \in \mathcal{M} \\ D_m = D}} S_m, \quad \text{and} \quad \widehat{D} \in \underset{D \in \mathbb{N}}{\text{argmin}} \{ \widehat{\mathcal{R}}_n(\widehat{s}'_D) + \text{pen}(D) \}.$$

Then, discarding all models of dimension  $D > n$ ,  $\widehat{s}_{\widehat{m}} = \widehat{s}'_{\widehat{D}}$  is a penalized empirical risk minimizer over a collection  $(S'_D)_{0 \leq D \leq n}$  of cardinality at most  $n + 1$ . The difference with the initial formulation is that the models  $S'_D$  are not vector spaces (in general), and the complexity of  $S'_D$  strongly depends on  $f(D) := \text{card}\{m \in \mathcal{M} / D_m = D\}$ . Three cases can be distinguished, following Birgé and Massart (2007):

- (i)  $\mathcal{M}$  is “small” or “polynomial” when  $f(D) \leq CD^\omega$  for some  $C, \omega > 0$ . Then,  $\text{card}(\mathcal{M})$  grows polynomially with  $n$  (since models of dimension  $D_m > n$  can safely be discarded), and the complexity of  $S'_D$  is essentially the same as the one of a  $D$ -dimensional vector space.

- (ii)  $\mathcal{M}$  is “large” or “exponential” when  $f(D)$  grows much faster —typically of order  $\binom{n}{D}$ —, which implies in particular that  $\text{card}(\mathcal{M})$  grows exponentially with  $n$ . Then,  $S'_D$  is much more complex than a  $D$ -dimensional vector space. A typical example is (full) variable selection among  $p \geq n$  variables, for which  $f(D) = \binom{p}{D} \geq \binom{n}{D}$ .
- (iii)  $\mathcal{M}$  is “moderate” in the intermediate situation, when  $D^{-1} \log f(D)$  stays bounded away from 0 and  $\infty$  for  $n \gg D \gg 1$ .

The current subsection focuses on cases (ii) and (iii); all other results mentioned in this article correspond to case (i).

#### *Results for case (ii): large number of models*

In fixed-design regression with least-squares risks and estimators,  $(\beta')$  and  $(\tilde{\gamma})$  are proved by [Birgé and Massart \(2007\)](#) for the (full) variable-selection problem with  $p$  orthonormal variables, assuming that the noise is Gaussian, and defining

$$\text{pen}_0(m) = \frac{D_m}{n} \left( 1 + 2 \log \frac{p}{D_m} \right), \quad C^* = \sigma^2,$$

and  $\text{pen}_1(m) = C \text{pen}_0$  with any  $C > 1$ . Note that  $(\beta^-)$  can be derived from the proof by [Birgé and Massart \(2007\)](#), Proposition 2), but it is not written in the article by [Birgé and Massart \(2007\)](#).

Similar theoretical results are proved by [Sorba \(2017\)](#), Chapter 8) for Gaussian variable selection with  $p = n$  and a more general collection of models, that can be smaller than full variable selection but still exponentially large. Formally, [Sorba \(2017\)](#), Section 8.1) assumes that  $\mathcal{M}$  satisfies a “completion rule”, which holds for instance for the collection of regressograms over a partition whose cells are hyperrectangles of  $\mathbb{R}^d$ . Then,  $(\beta'^-)$  and  $(\tilde{\gamma})$  hold true, with  $\text{pen}_0(m)$  proportional to  $\frac{D_m}{n} \log \frac{en}{D_m}$  —showing that a  $\log(n)$  factor is still necessary here— and  $(\beta^-)$  is proved when the target signal is null. Compared to the results of [Birgé and Massart \(2007\)](#), a gap of a multiplicative constant remains between minimal and sufficient penalties.

[Sorba \(2017\)](#), Chapter 9) proves similar theoretical results about histogram selection for density estimation by penalized log-likelihood, with the Kullback risk, for any large collection of subpartitions of a regular partition of  $[0, 1]$  into  $N + 1$  pieces, assuming  $N \leq n/(\log n)^2$ . A sufficient penalty  $\propto \frac{D_m}{n} \log(N)$  satisfies  $(\tilde{\gamma})$ . If the target density is uniform over  $[0, 1]$ ,  $(\beta'^-)$  holds true with a minimal penalty level of the same order of magnitude. As a consequence, when  $\log(N) \sim \log(n)$ , this proves that a  $\log(n)$  factor must be added to the penalty compared to the case of a polynomial collection  $\mathcal{M}$ .

Two partial results are available with multiplicative penalties, which are introduced in Section 4.6. In the same setting as [Birgé and Massart \(2007\)](#),  $(\beta^-)$  —assuming  $s^* = 0$  and a specific “exponential” collection  $\mathcal{M}$  with  $f(D) \approx \binom{n}{D}$ —,  $(\beta'^+)$ , and  $(\tilde{\gamma})$  are proved by [Baraud et al. \(2009\)](#), with  $\text{pen}_0^{\text{mult}}(m) = 2D_m \log(n)$ . For estimation of a Gaussian graph —that is, in a Gaussian graphical model, predict the value at each vertex of the graph given its neighbors, by linear regression—, with least-squares risk and estimators,  $(\beta^-)$  —assuming that  $s^* = 0$  and  $\mathcal{M}$  contains some specific “exponential” collection with  $f(D) \approx \binom{p}{D}$  for some  $p > n$ —,  $(\beta'^+)$ , and  $(\tilde{\gamma})$  are proved by [Giraud \(2008\)](#), with  $\text{pen}_0^{\text{mult}}(m) = 2D_m \log(p)$ . In both articles by [Baraud et al. \(2009\)](#) and [Giraud \(2008\)](#),  $(\tilde{\gamma})$  holds with  $\text{pen}_1^{\text{mult}} = C \text{pen}_0^{\text{mult}}$  for any  $C > 1$ .

Finally, several other arguments can be found for the necessity of a penalty larger than

$$\sigma^2 \frac{D_m}{n} \left( 1 + \log \frac{n}{D_m} \right)$$

—up to a numerical constant— for change-point detection, which is an instance of variable selection with  $p = n - 1$ . Minimax lower bounds (Durot et al., 2009, Theorem 2) and general oracle inequalities (Birgé and Massart, 2007) prove that for the true model  $m^*$ ,

$$\text{pen}(m^*) \geq \kappa \sigma^2 \frac{D_{m^*}}{n} \left( 1 + \log \frac{n}{D_{m^*}} \right)$$

is necessary for some constant  $\kappa > 0$ . Abramovich et al. (2006, Section 1.9) provide several other reasons why the optimal penalty should be close to  $2\sigma^2 \frac{D_m}{n} \log \frac{n}{D_m}$ .

*Results for case (iii): moderate number of models*

In fixed-design regression with least-squares risks and estimators,  $(\tilde{\gamma})$  holds true in general, and  $(\tilde{\beta}')$  is proved assuming that  $s^* = 0$  and all models of the same dimension  $D$  are orthogonal (Birgé and Massart, 2007, Proposition 3), with

$$\text{pen}_0(m) = \lambda \frac{D_m}{n} \left[ 1 + 2\sqrt{f(D_m)} + 2f(D_m) \right], \quad f(D) = a + \frac{b \log(D+1)}{D}, \quad \text{and} \quad C^* = \sigma^2$$

under some condition on the constants  $\lambda, a, b$ . By  $(\tilde{\beta}')$ , we mean  $(\tilde{\beta})$  with a jump in the risk instead of the complexity; here, the gap in  $(\tilde{\beta}')$  is  $C_2^*/C_1^* = 6/5$ .

Results of the same flavor exist for a toy problem close to the above setting (Sorba, 2017, Chapter 10), and for a Gaussian linear process and a  $b$ -ary tree partition collection —with no assumption on  $s^*$  for proving  $(\beta^-)$  and  $(\beta'^-)$ — (Sorba, 2017, Chapter 6). All these results show that “intermediate” collections of models can require a penalty strictly larger than the minimal penalty  $\frac{\sigma^2 D_m}{n}$  of “polynomial” collections.

## 5. Towards new theoretical results on minimal penalties

We now describe some strategies for proving that Algorithm 5 works in other settings. This section is a bit more abstract and technical than the rest of the article, so it can be skipped at first reading. As in Section 4.1, whose notation is used throughout the section, we consider separately subproblems  $(\alpha)$ ,  $(\beta)$ , and  $(\gamma)$ .

### 5.1. Hints for $(\alpha)$ : how to find $\text{pen}_0$ , $\text{pen}_1$ , and $\mathcal{C}_m$ ?

Using the notation defined by Eq. (55), (56), and (57), Section 3.6 suggests that  $p_1(m) + p_2(m)$  or its expectation  $\text{pen}_{\text{opt}}^{\text{gal}}(m)$  should be an optimal penalty, and  $p_2(m)$  or its expectation  $\text{pen}_{\text{min}}^{\text{gal}}(m)$  should be a minimal penalty.

In both cases, computing (approximately)  $\mathbb{E}[p_i(m)]$ ,  $i = 1, 2$ , or deriving an asymptotic expansion of  $p_i(m)$ ,  $i = 1, 2$ , at least for  $\mathcal{C}_m$  large enough, can lead to formulas for  $\text{pen}_0(m)$  and

$\text{pen}_1(m)$ . For instance, for fixed-design regression with the least-squares risk, exact formulas for  $\mathbb{E}[p_i(m)]$  lead to Algorithm 1 for least-squares estimators, and to Algorithm 4 for linear estimators. The main difficulty here is to have no unknown quantity inside  $\text{pen}_0$  or  $\text{pen}_1$ .

For general estimators in the fixed-design regression setting, an exact formula for  $\text{pen}_{\text{opt}}^{\text{gal}}(m)$  is given by covariance penalties (Efron, 2004), which can be expressed using the degrees of freedom when the noise is Gaussian and the loss is quadratic. For maximum-likelihood estimators and risk, a partial asymptotic solution is given by the formula of the AIC criterion (Akaike, 1973), which derives from some version of the Wilks phenomenon (see also Section 5.2). In both cases, only a formula for  $\text{pen}_1$  is available, and  $\text{pen}_0$  remains unknown, even if one can sometimes conjecture that  $\text{pen}_0 = \text{pen}_1 / 2$ .

For random-design regression with the quadratic risk, Navarro and Saumard (2017, Theorem 6.3) provide an (approximate) closed-form formula for  $\mathbb{E}[p_1(m)]$  and  $\mathbb{E}[p_2(m)]$  —by proving that  $p_1(m)$  and  $p_2(m)$  concentrate around some deterministic quantity, which is not necessarily equal to their expectation— that is not directly useful because it depends on the unknown distribution of the  $(X_i, Y_i)$ .

Another option is to define  $\text{pen}_0(m)$ , resp.  $\text{pen}_1(m)$ , as some resampling-based estimator of  $\mathbb{E}[p_2(m)]$ , resp.  $\mathbb{E}[p_2(m) + p_1(m)]$ , and to use Algorithm 5 for estimating the common (unknown) multiplicative factor  $C^*$  such that

$$C^* \mathbb{E}[\text{pen}_0(m)] \approx \mathbb{E}[p_2(m)] \quad \text{and} \quad C^* \mathbb{E}[\text{pen}_1(m)] \approx \mathbb{E}[p_1(m) + p_2(m)],$$

see Remark 3 in Section 4.2. In addition to the papers mentioned in Section 4.2, let us mention here that a concentration result for the resampling estimate of  $\mathbb{E}[p_2(m)]$  is proved by Arlot (2007, Chapter 7), for empirical risk minimizers and a general bounded risk.

If no natural quantity arises as a complexity measure  $\mathcal{C}_m$ , such as the number of parameters in regression,  $\mathbb{E}[p_2(m)]$  (or a resampling-based estimator of it) can be a good guess for  $\mathcal{C}_m$ , see the article by Lerasle (2012) and Remark 3.

## 5.2. Hints for $(\beta)$ : how to prove that $C^* \text{pen}_0$ is a minimal penalty?

Following the results mentioned in the previous subsections, two general approaches can be used for proving  $(\beta)$ , assuming either that  $C^* \text{pen}_0(m) = \mathbb{E}[p_2(m)]$  as in Theorem 1, or that  $\text{pen}_0(m) = \mathcal{C}_m = p_2(m)$  as done by Lerasle and Takahashi (2016). This section details these two approaches for proving  $(\beta^-)$  and  $(\beta^+)$ , before focusing on the concentration inequalities they both require. Recall that

$$\forall C \geq 0, \quad \hat{m}_{\min}^{(0)}(C) \in \underset{m \in \mathcal{M}}{\text{argmin}} \left\{ \hat{\mathcal{R}}_n(\hat{s}_m) + C \text{pen}_0(m) \right\}.$$

### 5.2.1. Below the minimal penalty: ( $\beta^-$ )

**Following the proof of Theorem 1** When  $C^* \text{pen}_0(m) = \mathbb{E}[p_2(m)]$ , similarly to the proof of Eq. (14) in Theorem 1, one can prove ( $\beta^-$ ) by showing that for some well-chosen  $m_1 \in \mathcal{M}$ ,

$$\forall C < (1 - \eta_n^-)C^*, \quad \inf_{m \in \mathcal{M} / \mathcal{C}_m < \mathcal{C}_{\text{overfit}}} G_C(m) > G_C(m_1)$$

$$\text{where } G_C(m) := \widehat{\mathcal{R}}_n(\widehat{s}_m) + C \text{pen}_0(m) = \mathcal{R}(s_m^*) - \delta(m) - p_2(m) + \frac{C}{C^*} \mathbb{E}[p_2(m)]$$

is the quantity minimized by  $\widehat{m}_{\min}^{(0)}(C)$ . Then, in addition to the arguments sketched in Section 3.5, we only need here tight concentration inequalities for  $\delta(m) - \delta(m_1)$  and for  $p_2(m)$ , see Section 5.2.3. A natural choice for  $m_1$  is a minimizer of the approximation error  $\mathcal{R}(s_m^*) - \mathcal{R}(s^*)$  over  $m \in \mathcal{M}$ .

### Generalizing the strategy of Lerasle and Takahashi (2016) and Garivier and Lerasle (2011)

When  $\text{pen}_0(m) = \mathcal{C}_m \propto p_2(m)$ , the approach<sup>3</sup> used by Lerasle and Takahashi (2016) and Garivier and Lerasle (2011) can be summarized into the following proposition.

**Proposition 1.** *Let us consider the general framework of Section 3.1 and use the notation of Section 4.1. Let  $\varepsilon_\delta \in [0, 1]$ ,  $\varepsilon'_\delta \geq 0$ , and assume that for every  $m \in \mathcal{M}$ ,  $\text{pen}_0(m) = p_2(m)$  and*

$$\forall m, m' \in \mathcal{M}, \quad |\delta(m) - \delta(m')| \leq \varepsilon_\delta [\mathcal{R}(s_m^*) - \mathcal{R}(s^*) + \mathcal{R}(s_{m'}^*) - \mathcal{R}(s^*)] + \varepsilon'_\delta. \quad (60)$$

Then, for every  $C \in [0, 1)$ ,

$$p_2(\widehat{m}_{\min}^{(0)}(C)) \geq \sup_{m \in \mathcal{M}} \left\{ p_2(m) - \frac{2}{1-C} [\mathcal{R}(s_m^*) - \mathcal{R}(s^*)] \right\} - \frac{\varepsilon'_\delta}{1-C}, \quad (61)$$

and if  $\mathcal{R}(s_{m_1}^*) = \mathcal{R}(s^*)$  for some  $m_1 \in \mathcal{M}$  with  $p_2(m_1) > 0$ , for any  $\alpha \in (0, 1)$ ,

$$\forall C \leq 1 - \eta_\alpha, \quad p_2(\widehat{m}_{\min}^{(0)}(C)) \geq (1 - \alpha)p_2(m_1) \quad \text{with} \quad \eta_\alpha = \frac{\varepsilon'_\delta}{\alpha p_2(m_1)}. \quad (62)$$

Assume in addition that the data  $\xi_1, \dots, \xi_n \in \mathcal{X}$  are i.i.d. and some contrast function  $\gamma : \mathbb{E} \times \mathbb{S} \rightarrow \mathbb{R}$  and constants  $A, L > 0$  exist such that

$$\forall t \in \mathbb{S}, \quad \widehat{\mathcal{R}}_n(t) = \frac{1}{n} \sum_{i=1}^n \gamma(\xi_i, t) \quad \text{and} \quad \mathcal{R}(t) = \mathbb{E}[\widehat{\mathcal{R}}_n(t)] = \mathbb{E}[\gamma(\xi_1, t)], \quad (63)$$

$$\forall t \in \mathbb{S}, \quad |\gamma(\xi_1, t)| \leq A \quad \text{a.s.}, \quad (64)$$

$$\text{and} \quad \forall m \in \mathcal{M}, \quad \text{var}(\gamma(\xi_1, s_m^*) - \gamma(\xi_1, s^*)) \leq L[\mathcal{R}(s_m^*) - \mathcal{R}(s^*)]. \quad (65)$$

Then, for every  $x \geq 0$ , with probability at least  $1 - 2 \text{card}(\mathcal{M})e^{-x}$ , for any  $\theta > 0$ , Eq. (60) holds true with

$$\varepsilon_\delta = \theta \quad \text{and} \quad \varepsilon'_\delta = \left( \frac{L}{\theta} + \frac{4A}{3} \right) \frac{x}{n}.$$

<sup>3</sup> It should be noticed here that the article by Lerasle and Takahashi (2016) was prepublished on June 2011 (arXiv preprint number 1106.2467), a few months before the preprint by Garivier and Lerasle (2011), despite what the publication date of the former paper suggests.

Proposition 1 is proved in Appendix A.1. Eq. (62) proves that  $(\beta^-)$  holds true if  $p_2(m_1)$  is close to  $\sup_{m \in \mathcal{M}} p_2(m)$ , which is a reasonable assumption. For instance, in the setting of Section 2,  $m_1$  is given by assumption (HId) leading to  $\hat{s}_{m_1} = Y$ , hence

$$p_2(m_1) = \frac{1}{n} (\|Y - F_{m_1}\|^2 - \|Y - \hat{F}_{m_1}\|^2) = \frac{1}{n} \|\varepsilon\|^2 \approx \sigma^2.$$

The proof of Proposition 1 also works when assuming only that  $p_2(m) \geq 0$  for every  $m \in \mathcal{M}$  and

$$(1 - \varepsilon_0)p_2(m) \leq \text{pen}_0(m) \leq (1 + \varepsilon_0)p_2(m),$$

which can be used when  $\text{pen}_0(m)$  is a resampling estimate of  $\mathbb{E}[p_2(m)]$  for instance. Then, we loose a factor in the “rate”  $\eta_\alpha$  of estimation of  $C^*$  in Eq. (62), see Appendix A.1.

Proposition 1 is new —apart from the fact that its proof relies heavily on the proof technique proposed by Lerasle and Takahashi (2016)— but rather abstract in its general form. Under the additional conditions (63)–(65), it can be used for minimum-contrast estimators

$$\hat{s}_m \in \underset{t \in S_m}{\text{argmin}} \{ \hat{\mathcal{R}}_n(t) \}$$

with a bounded contrast  $\gamma$ , so that one automatically has  $p_2(m) \geq 0$  and Eq. (63)–(64) as requested. Then, Eq. (65) is a classical assumption (Massart and Nédélec, 2006) which holds for bounded regression with the least-squares contrast —with  $L = A = 8M^2$  if data are bounded by  $M$ , according to Arlot and Massart (2009)—, and for binary classification with the 0–1 loss under the margin condition (Mammen and Tsybakov, 1999; Massart and Nédélec, 2006). Let us emphasize that Algorithm 5 has never been justified for binary classification with the 0–1 loss up to now, so Proposition 1 is of significant interest even if it only provides a partial justification —with  $(\beta^-)$  only, in a rather abstract form.

### 5.2.2. Above the minimal penalty: $(\beta^+)$

Before detailing two approaches for proving  $(\beta^+)$ , let us recall that if an oracle inequality like  $(\beta'^+)$  is available, a simple way to prove  $(\beta^+)$  is to use the connection from  $(\beta'^+)$  to  $(\beta^+)$  explained in Section 4.4.

**Following the proof of Theorem 1** When  $C^* \text{pen}_0(m) = \mathbb{E}[p_2(m)]$ , following the proof of Eq. (16) in Theorem 1,  $(\beta^+)$  can be proved by showing that for some well-chosen  $m_2 \in \mathcal{M}$ ,

$$\forall C > (1 + \eta_n^+)C^*, \quad \inf_{m \in \mathcal{M} / \mathcal{C}_m > \mathcal{C}_{\text{small}}} G_C(m) > G_C(m_2),$$

which requires concentration inequalities for  $\delta(m) - \delta(m_2)$  and for  $p_2(m)$ , see Section 5.2.3. Two natural choices are

$$m_2 \in \underset{m \in \mathcal{M} / \mathcal{C}_m \leq \mathcal{C}_{\text{small}}}{\text{argmin}} \{ \mathcal{R}(s_m^*) - \mathcal{R}(s^*) \} \quad \text{and} \quad m_2 \in \underset{m \in \mathcal{M}}{\text{argmin}} \left\{ \mathbb{E}[\mathcal{R}(\hat{s}_m) - \mathcal{R}(s^*)] \right\}.$$



**Generalizing the strategy of Lerasle and Takahashi (2016) and Garivier and Lerasle (2011)**

When  $\text{pen}_0(m) = \mathcal{C}_m \propto p_2(m)$ , the approach used by Lerasle and Takahashi (2016) and Garivier and Lerasle (2011) can be summarized into the following proposition.

**Proposition 2.** *Let us consider the general framework of Section 3.1 and use the notation of Section 4.1. Let  $\varepsilon_\delta, \varepsilon_p \in [0, 1]$ ,  $\varepsilon'_\delta \geq 0$ , assume that Eq. (60) holds true and that for every  $m \in \mathcal{M}$ ,  $\text{pen}_0(m) = p_2(m)$  and*

$$|p_1(m) - p_2(m)| \leq \varepsilon_p p_1(m). \quad (66)$$

Then, for every  $C > 1$ , we have

$$\mathcal{R}(\widehat{s}_{\widehat{m}_{\min}^{(0)}(C)}) - \mathcal{R}(s^*) \leq K(C) \inf_{m \in \mathcal{M}} \{\mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*)\} + K'(C) \quad (67)$$

$$\text{and } p_2(\widehat{m}_{\min}^{(0)}(C)) \leq K(C)(1 + \varepsilon_p) \inf_{m \in \mathcal{M}} \{\mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*)\} + K'(C)(1 + \varepsilon_p), \quad (68)$$

$$\text{where } K(C) := \frac{\max\{(C-1)(1+\varepsilon_p), 1+\varepsilon_\delta\}}{\min\{(C-1)(1-\varepsilon_p), 1-\varepsilon_\delta\}}$$

$$\text{and } K'(C) := \frac{\varepsilon'_\delta}{\min\{(C-1)(1-\varepsilon_p), 1-\varepsilon_\delta\}}.$$

Proposition 2 is proved in Appendix A.2.

Now, assume that Eq. (60) and (66) hold on a large-probability event. Then, taking  $C = 1 + \eta$  with  $\eta > 0$ , we get  $K(C) \leq \mathcal{O}(1)/\eta$  if  $\eta$  is small enough, and Eq. (67) implies  $(\beta^{++})$ . If in addition  $p_2(m_1)$  stays bounded away from zero as  $n$  tends to infinity, Eq. (62) implies  $(\beta^-)$ . If moreover the oracle risk tends to zero and  $\varepsilon'_\delta = o(1)$ , then, Eq. (68) implies  $(\beta^+)$ . Assuming also that  $\max\{\varepsilon_\delta, \varepsilon_p\} = o(1)$ , then  $K(2) = 1 + o(1)$  hence Eq. (67) with  $C = 2$  implies a first-order optimal oracle inequality  $(\gamma)$  with  $\text{pen}_1 = 2\text{pen}_0$ .

The conditions of Proposition 2 can be relaxed. First,  $\text{pen}_0(m) = p_2(m)$  can be replaced by  $(1 - \varepsilon_0)p_2(m) \leq \text{pen}_0(m) \leq (1 + \varepsilon_0)p_2(m)$  for some  $\varepsilon_0 \geq 0$  with  $C(1 - \varepsilon_0) > 1$ , which can be used when  $\text{pen}_0(m)$  is a resampling estimate of  $\mathbb{E}[p_2(m)]$  for instance. Second, Eq. (66) can be replaced by  $\forall m \in \mathcal{M}$ ,  $-\varepsilon'_p + \varepsilon_p^- p_1(m) \leq p_2(m) \leq \varepsilon_p^+ p_1(m) + \varepsilon'_p$  for some  $\varepsilon_p^-, \varepsilon_p^+ > 0$  and  $\varepsilon'_p \geq 0$ . Then,  $K(C)$  and  $K'(C)$  are slightly enlarged, as well as the bound in Eq. (68), see Appendix A.2. In particular, Proposition 2 can justify  $(\gamma)$  with  $\text{pen}_1 = (1 + \alpha^{-1})\text{pen}_0$  provided that both  $\varepsilon_p^-$  and  $\varepsilon_p^+$  converge to  $\alpha > 0$ , and  $\varepsilon'_p$  is small enough.

Assumption (66) is strong and we do not expect that it can be proved as generally as assumption (60) in Proposition 1. Nevertheless, it holds when  $p_1(m)$  and  $p_2(m)$  both concentrate around  $\mathbb{E}[p_1(m)] \approx \mathbb{E}[p_2(m)]$  for every  $m \in \mathcal{M}$ , and it can be satisfied in other cases. For instance, for least-squares estimators in least-squares fixed-design regression (Section 2) or in least-squares density estimation (Lerasle, 2012),  $p_1(m) = p_2(m)$  almost surely. Bounding  $|p_1(m) - p_2(m)|$  also turns out to be easier to get than a concentration inequality for  $p_1$  and  $p_2$  separately in some settings where  $p_1(m) \neq p_2(m)$  in general (Garivier and Lerasle, 2011).

Whatever the proof technique used —through  $(\beta^{++})$ , as in the proof of Theorem 1 or as in the article by Lerasle and Takahashi (2016)—, proving that the upper bound on the complexity in  $(\beta^+)$  is much smaller than the lower bound in  $(\beta^-)$  is done by assuming that the oracle risk



tends to zero as  $n \rightarrow \infty$ , or at least that some estimator of “not too large” complexity has a small approximation error (as in Theorem 1). We conjecture that such an assumption is unavoidable in general.

### 5.2.3. Concentration inequalities

The proof techniques summarized in Sections 5.2.1–5.2.2 require some concentration inequalities for  $\delta(m) - \delta(m')$  and  $p_2(m)$ , and some deviation inequalities for  $|p_1(m) - p_2(m)|/p_1(m)$ . This section provides some ways to obtain such results.

**Concentration of  $\delta(m) - \delta(m')$**  As explained in the proof of Proposition 1,  $\delta(m) - \delta(m')$  is a sum of independent and identically distributed random variables, so it can be concentrated with Bernstein’s inequality (Boucheron et al., 2013, Theorem 2.10), leading to a result like Eq. (60) if a boundedness assumption (64) and some margin-type condition (65) are satisfied.

In the unbounded case, other kinds of concentration inequalities can be used. For instance, for density estimation with the Kullback risk and maximum-likelihood estimators on histogram models—that is, the setting of Saumard (2010c) without the boundedness assumption on the target density—, Saumard and Navarro (2018, Sections 4.2–4.3) use a modified version of Bernstein’s inequality for controlling  $\delta(m) - \delta(m')$ . Note that Saumard and Navarro (2018) only prove  $(\beta^+)$  and a first-order optimal oracle inequality  $(\gamma)$ , but the proofs of Saumard and Navarro (2018) can be adapted to get a full proof of the slope heuristics, that is, a result similar to the one of Saumard (2010c) when the density can be unbounded.

**Concentration of  $p_2(m)$**  The problem is much harder for  $p_2(m)$ . It can be seen as proving a non-asymptotic version of the Wilks phenomenon (Wilks, 1938) in a nonparametric setting with model misspecification (Boucheron and Massart, 2011), which makes this problem interesting beyond minimal-penalty algorithms. In addition to the settings mentioned in Section 4.2, concentration results for  $p_2$  are available in two cases.

For bounded-contrast minimizers, a concentration inequality is proved in a general setting including bounded regression and classification with Vapnik-Chervonenkis classes (Boucheron and Massart, 2011). This result can be used for proving that Algorithm 5 works with regression estimators (Arlot and Massart, 2009).

For maximum-likelihood estimators, in a parametric setting (Spokoiny, 2012), in a semiparametric setting (Andresen and Spokoiny, 2014) and in a nonparametric setting with a quadratic penalty (Spokoiny, 2017),  $p_2$  is close to some quadratic form with high probability, and this quadratic form itself satisfies some concentration properties. Nevertheless, these results have not been used yet for proving that Algorithm 5 works.

Note also that a concentration inequality for  $p_2(m)$ , with histogram (maximum-likelihood) density estimators and the Kullback risk, have been obtained by Saumard and Navarro (2018), improving previous results by Saumard (2010c).

**Proof of Eq. (66)** Apart from the specific approaches mentioned in Section 5.2.2, we do not know any result for bounding directly  $|p_1(m) - p_2(m)|/p_1(m)$  as required in Eq. (66).

### 5.3. Hints for $(\gamma)$ : how to prove that $C^*$ $\text{pen}_1$ is an optimal penalty?

When  $C^* \text{pen}_1(m) = \mathbb{E}[p_1(m) + p_2(m)]$ , oracle inequalities  $(\gamma)$  or  $(\tilde{\gamma})$  usually rely on some concentration inequality for the ideal penalty  $\mathcal{R}(\hat{s}_m) - \hat{\mathcal{R}}_n(\hat{s}_m) = p_1(m) + \delta(m) + p_2(m)$ , as in step 3 of the proof of Theorem 1. One actually needs only concentration for

$$[\mathcal{R}(\hat{s}_m) - \hat{\mathcal{R}}_n(\hat{s}_m)] - [\mathcal{R}(\hat{s}_{m'}) - \hat{\mathcal{R}}_n(\hat{s}_{m'})]$$

for all  $m, m' \in \mathcal{M}$ . Concentration results for  $\delta(m) - \delta(m')$  and for  $p_2(m)$  are reviewed in Section 5.2 since they are usually required for proving  $(\beta)$ . Therefore, we now focus on  $p_1(m)$ .

**Concentration of the excess risk  $p_1(m)$**  What remains is to concentrate  $p_1(m)$  —or equivalently  $\mathcal{R}(\hat{s}_m) - \mathcal{R}(s^*)$  or  $\mathcal{R}(\hat{s}_m)$ — around its expectation, a difficult problem that has not been solved except in a few settings: the ones for which a full proof of the slope heuristics exists —see Section 4.2—, and the ones listed below.

Several papers recently tackled the case of fixed-design linear regression with the least-squares risk, when  $\hat{s}_m$  minimizes a (penalized) least-squares criterion over a convex set, assuming that the penalty  $\Omega$  is convex. Concentration inequalities for

$$\sqrt{\mathcal{R}(\hat{s}_m) - \mathcal{R}(s^*)} \quad \text{or} \quad \sqrt{\mathcal{R}(\hat{s}_m) - \mathcal{R}(s^*) + \Omega(\hat{s}_m)}$$

are available under different assumptions on the noise (Gaussian or not) and on  $\Omega$  (Chatterjee, 2014; Bellec, 2017; Bellec and Tsybakov, 2017; Muro and Geer, 2018). They apply to various examples such as the Lasso (in its constrained formulation) and isotonic regression (Chatterjee, 2014), the Lasso and the group Lasso in their usual regularization formulation (Bellec, 2017; Bellec and Tsybakov, 2017), splines and total-variation regularization (Muro and Geer, 2018). When  $\Omega$  is a semi-norm, Bellec (2018) proves upper and lower bounds on  $\mathbb{E}[\mathcal{R}(\hat{s}_m)]$ . The article by Chen et al. (2017) also is related to this topic.

For general losses, high-probability upper and lower bounds on  $\mathcal{R}(\hat{s}_m) - \mathcal{R}(s^*)$  —sometimes plus a regularization term  $\Omega(\hat{s}_m)$ — are proved by Bartlett and Mendelson (2006) for general empirical minimizers —with a rather abstract result—, by Saumard (2010b) for “regular” estimators and losses, and by van de Geer and Wainwright (2017) for regularized empirical risk minimizers —with precise applications provided for “linear losses” such as linearized least-squares regression, maximum-likelihood estimators on an exponential model, and log-linear regression. Note that the general approaches of Bartlett and Mendelson (2006), Saumard (2010b) and van de Geer and Wainwright (2017) are closely related; Chatterjee (2014), Bellec (2017), Bellec and Tsybakov (2017) and Muro and Geer (2018), which are mentioned above for linear regression, use a similar technique that is exposed clearly by Bellec (2017, Section 2) for instance.

Saumard (2017) proves a concentration inequality for the quadratic risk  $\mathcal{R}(\hat{s}_m)$  of a least-squares estimator over a convex set, in the heteroscedastic random-design regression setting; this result requires to handle specifically the quadratic part of the empirical process, which cannot be concentrated tightly with the general approach of van de Geer and Wainwright (2017) for instance. Note also that the result obtained by Saumard (2017) applies to more general models than the ones of Navarro and Saumard (2017) for which a full proof of the slope heuristics exist.

For histogram (maximum-likelihood) estimators and the Kullback risk in density estimation, in addition to the result obtained by [Saumard \(2010c\)](#) and mentioned in Section 4.2, concentration inequalities for  $\mathcal{R}(\hat{s}_m)$  have been obtained by [Castellan \(1999\)](#), and [Saumard and Navarro \(2018\)](#) have recently improved them.

Let us also recall that Proposition 2 in Section 5.2.2 provides an alternative approach for proving  $(\gamma)$  when  $\text{pen}_1(m) \propto p_2(m)$ .

## 6. Related procedures

Minimal-penalty algorithms are primarily made for model/estimator selection, but in the fixed-design regression setting (Algorithms 1 and 4) they also provide an estimator  $\hat{C}_{\text{jump}}$  of the noise variance  $\sigma^2$ . This section compares minimal penalties to its main alternatives for both tasks, starting by residual-(co)variance estimation.

### 6.1. Residual-variance estimation

Let us consider the fixed-design regression setting of Sections 2 and 3.3–3.4 and their notation. An example of interest is when

$$\forall i \in \{1, \dots, n\}, \quad F_i = f(x_i) \quad \text{for some smooth } f \text{ and some design points } x_i \in \mathbb{R}^d. \quad (69)$$

**Literature on residual-variance estimation** Many estimators exist for the residual variance  $\sigma^2$  in nonparametric regression. An exhaustive list is beyond the scope of this article; for more references, we refer to the articles by [Hall et al. \(1990\)](#), [Dette et al. \(1998\)](#), [Spokoiny \(2002\)](#), [Müller et al. \(2003\)](#), [Liitiäinen et al. \(2009\)](#) and [Ramosaj and Pauly \(2019\)](#), and to the articles by [Belloni et al. \(2014\)](#), [Chatterjee \(2015\)](#), [Reid et al. \(2016\)](#) and [Giacobino et al. \(2017\)](#) for the high-dimensional variable-selection case. A related problem is noise-variance estimation in heteroscedastic regression (see [Brown and Levine, 2007](#), [Gendre, 2008](#), and references therein).

This section focuses on minimal-penalty based estimators and on estimators that are quadratic forms of the data vector  $Y \in \mathbb{R}^n$ , that is,

$$\hat{\sigma}_B^2 := \frac{\langle Y, BY \rangle}{\text{tr}(B)} \quad (70)$$

where  $B$  is some  $n \times n$  symmetric matrix. Eq. (70) actually covers several, if not all, classical residual-variance estimators—in particular the ones suggested in the context of model/estimator selection with  $C_p$  or  $C_L$ —, which allows their common non-asymptotic analysis ([Dette et al., 1998](#)).

**Residual-based estimators** The most classical variance estimators are based upon the residuals—through the empirical risk— on some model  $S_{m_0}$  :

$$\hat{\sigma}_{m_0}^2 := \frac{1}{n - D_{m_0}} \|Y - \hat{F}_{m_0}\|^2. \quad (71)$$

Remark that  $\widehat{\sigma}_{m_0}^2 = \widehat{\sigma}_B^2$  with  $B = I_n - \Pi_{m_0}$ . When  $\sigma^2$  must be estimated in the formula of the  $C_p$  penalty, the classical suggestions are of the form  $\widehat{\sigma}_{m_0}^2$  (Mallows, 1973; Efron, 1986; Baraud, 2000).

The bias of  $\widehat{\sigma}_{m_0}^2$  as an estimator of  $\sigma^2$  can be derived from Eq. (8):

$$\mathbb{E}[\widehat{\sigma}_{m_0}^2] - \sigma^2 = \frac{1}{n - D_{m_0}} \|(I_n - \Pi_{m_0})F\|^2. \quad (72)$$

If  $F \in S_{m_0}$ , then  $\widehat{\sigma}_{m_0}^2$  is unbiased, and otherwise it suffers some upward bias, depending on the approximation error and on the dimension of  $S_{m_0}$ . Proposition 4 in Appendix A.4 provides a general formula for the variance and MSE of  $\widehat{\sigma}_{m_0}^2$ . For instance, assuming for simplicity that the noise is Gaussian,

$$\mathbb{E}\left[(\widehat{\sigma}_{m_0}^2 - \sigma^2)^2\right] = \frac{2\sigma^4}{n - D_{m_0}} + \frac{4\sigma^2 \|(I_n - \Pi_{m_0})F\|^2}{(n - D_{m_0})^2} + \frac{\|(I_n - \Pi_{m_0})F\|^4}{(n - D_{m_0})^2}. \quad (73)$$

Choosing the model  $S_{m_0}$  without prior knowledge is a difficult question. For minimizing the MSE, one must trade off terms depending on  $1/(n - D_{m_0})$  and on the approximation error, that vary differently as functions of  $S_{m_0}$ ; this can be as difficult as the model-selection problem. When some unbiased model  $S_{m_0}$  is known with  $D_{m_0} = o(n)$ , taking it for the estimation of  $\sigma^2$  is a reasonable choice. This matches the suggestion of Mallows (1973) and Efron (1986) in the variable-selection setting with a full model of dimension  $p = o(n)$ . In the setting given by Eq. (69), when contiguous  $x_i$  are close enough, a natural choice for  $S_{m_0}$  is the linear span of  $(e_{2i} + e_{2i-1})_{1 \leq i \leq n/2}$  where  $(e_1, \dots, e_n)$  denotes the canonical basis of  $\mathbb{R}^n$ . Then, assuming for simplicity that  $n$  is even,

$$\widehat{\sigma}_{m_0}^2 = \frac{1}{n} \sum_{i=1}^{n/2} (Y_{2i} - Y_{2i-1})^2 \quad (74)$$

is a consistent estimator of  $\sigma^2$  if  $f$  is uniformly continuous and  $\max_{1 \leq i \leq n} \|x_i - x_{i+1}\| = o(1)$ .

Note that for high-dimensional variable selection, several residual-based estimators on a data-driven model  $m_0$  —for instance, chosen by cross-validation— are available, but theoretical guarantees are still lacking for several of them (Reid et al., 2016; Giacobino et al., 2017).

**Variance estimation with minimal penalties** The problem of choosing  $m_0$  for  $\widehat{\sigma}_{m_0}^2$  can be solved (bypassed in fact) by using the slope heuristics. Let us state non-asymptotic risk bounds for  $\widehat{C}_{\text{thr}}$  and  $\widehat{C}_{\text{window}}$  as estimators of  $\sigma^2$ , that derive from Theorem 1 and its proof in Section 2.

**Proposition 3.** *In the framework described in Section 2.1, assume that  $\mathcal{M}$  is finite, contains at least one model of dimension at most  $c_n \in [0, n/3)$ , and that (Hid) and (HG) hold true —see Section 2.5. Let  $\widehat{C}_{\text{thr}}(T_n)$  be defined by Eq. (20) with  $T_n \in (c_n, n)$ , and  $\widehat{C}_{\text{window}}(\eta)$  be defined by*

Eq. (19) with  $\eta > 0$ . For any  $x \geq 0$  and  $T \in (c_n, n)$ , let us define

$$\begin{aligned} C_1(x; T) &:= \sigma^2 \left( 1 - \frac{4\sqrt{\frac{x}{n}} + 6\frac{x}{n}}{1 - \frac{T}{n}} \right) \\ \text{and} \quad C_2(x; T; c_n) &:= \sigma^2 \left[ 1 + \frac{4n}{T - c_n} \left( \sqrt{\frac{x}{n}} + \frac{2x}{n} \right) \right] + \frac{2n}{T - c_n} \mathcal{B}(c_n) \\ \text{where} \quad \mathcal{B}(c_n) &:= \inf_{m \in \mathcal{M} / D_m \leq c_n} \left\{ \frac{1}{n} \| (I_n - \Pi_m) F \|^2 \right\}. \end{aligned}$$

Then, an event  $\Omega_x$  of probability at least  $1 - 4 \text{card}(\mathcal{M}) e^{-x}$  exists on which

$$\frac{C_1(x; \frac{2n}{3})}{1 + \eta} \leq \widehat{C}_{\text{window}}(\eta) \leq C_2(x; \frac{n}{3})(1 + \eta) \quad \text{if } \eta > \sqrt{\frac{C_2(x; \frac{n}{3})}{C_1(x; \frac{2n}{3})} - 1} \text{ and } x \in \left[ 0, \frac{n}{180} \right], \quad (75)$$

$$\text{and} \quad C_1(x; T_n) \leq \widehat{C}_{\text{thr.}}(T_n) \leq C_2(x; T_n; c_n). \quad (76)$$

If we assume in addition that  $c_n \leq T_n/2$ , then,

$$\begin{aligned} \mathbb{E} \left[ (\widehat{C}_{\text{thr.}} - \sigma^2)^2 \right] &\leq 739 \max \left\{ \left( 1 - \frac{T_n}{n} \right)^{-2}, \left( \frac{T_n}{2n} \right)^{-2} \right\} \\ &\times \left[ \left( \mathcal{B} \left( \frac{T_n}{2} \right) \right)^2 + \frac{\sigma^4 \log(4 \text{card } \mathcal{M})}{n} + \sigma^4 \left( \frac{\log(4 \text{card } \mathcal{M})}{n} \right)^2 \right]. \end{aligned} \quad (77)$$

Proposition 3 is proved in Appendix A.3. Note that the constant 739 in Eq. (77) can be strongly reduced under mild additional assumptions, see Appendix A.3. Proposition 3 can also be extended to  $(\phi^2 \sigma^2)$ -sub-Gaussian noise, at the price of replacing  $x$  by  $L\phi^2 x$  in Eq. (75)–(76) and  $\log(4 \text{card } \mathcal{M})$  by  $L\phi^2 \log(4 \text{card } \mathcal{M})$  in Eq. (77), where  $L$  is a numerical constant; see Remark 1 in Section 2.5.

If  $\mathcal{B}(c_n)$  tends to 0 as  $n$  tends to  $+\infty$ —which is a mild assumption—, by Proposition 3 with  $x = 2 \log(n) + \log(4 \text{card } \mathcal{M})$ , we get that  $\widehat{C}_{\text{thr.}}(T_n)$  and  $\widehat{C}_{\text{window}}(\eta)$  estimate consistently  $\sigma^2$ , with deviation bounds of order

$$\mathcal{B}(c_n) + \sigma^2 \sqrt{\frac{\log(n) + \log(\text{card } \mathcal{M})}{n}},$$

provided that  $c_n \leq \tau n$  with  $\tau < 1/3$ ,

$$T_n = \rho n \quad \text{with } \rho \in (0, 1), \quad \text{and} \quad \sigma^2 \eta \propto \mathcal{B}(c_n) + \sigma^2 \sqrt{\frac{\log(n) + \log(\text{card } \mathcal{M})}{n}}.$$

These deviation bounds for  $\widehat{C}_{\text{thr.}}$  and  $\widehat{C}_{\text{window}}$  can be interpreted as an oracle inequality, since they coincide with the best possible risk of  $\widehat{\sigma}_{m_0}^2$  with  $D_{m_0} \leq c_n$ , without any prior knowledge except the choice of  $(S_m)_{m \in \mathcal{M}}$ . Indeed, Eq. (73) shows that when  $D_{m_0} \leq c_n \leq \tau n$  with  $\tau < 1$ , up to constants depending on  $\tau$  only,

$$\sqrt{\mathbb{E}[(\widehat{\sigma}_{m_0}^2 - \sigma^2)^2]} \gtrsim \frac{1}{n} \| (I_n - \Pi_{m_0}) F \|^2 + \frac{\sigma^2}{\sqrt{n}} \geq \mathcal{B}(c_n) + \frac{\sigma^2}{\sqrt{n}}.$$

The bound (77) on the mean squared error (MSE) of  $\widehat{C}_{\text{thr}}$  can be compared to the minimax optimal rate  $\propto n^{-\min\{1,8/d\}}$  for the MSE in the setting of Eq. (69) when  $f$  has a bounded second-order derivative (Spokoiny, 2002). Assuming that  $\log(\text{card } \mathcal{M}) = o(n^{1/9})$ , that the approximation error  $\mathcal{B}(c_n)$  is minimax optimal hence of order  $c_n^{-4/d}$ , and that  $c_n \leq \tau n$  with  $\tau < 1$ , we get that  $\widehat{C}_{\text{thr}}$  is optimal when  $d \geq 9$  up to constants and within a factor  $\log(\text{card } \mathcal{M})$  of the minimax risk when  $d \leq 8$ . Similar risk bounds can easily be obtained from Proposition 3 under different assumptions on the signal. For instance, when Eq. (69) holds true with  $f$  that is  $\alpha$ -Hölderian for some  $\alpha > 0$ , an approximation error of order  $D_m^{-2\alpha/d}$  can be obtained with local polynomials of maximal degree  $\lfloor \alpha \rfloor$ . We conjecture that these residual-variance estimation bounds are minimax-optimal up to logarithmic factors provided that  $(S_m)_{m \in \mathcal{M}}$  has a cardinality at most polynomial in  $n$  and achieves the minimax approximation error bounds. These consequences of Proposition 3 have the flavor of adaptive risk bounds derived from oracle inequalities (Birgé and Massart, 1997), which is new for residual-variance estimation to the best of our knowledge. Therefore, the additional  $\log(\text{card } \mathcal{M})$  factor—coming from the union bound over  $m \in \mathcal{M}$  and typically of order  $\log(n)$ —seems a mild price for the versatility of  $\widehat{C}_{\text{thr}}$  and  $\widehat{C}_{\text{window}}$ .

**Residual-based estimators vs. the slope heuristics** In addition to the risk bounds comparison above, we can compare the definition of  $\widehat{\sigma}_{m_0}^2$  with the one of  $\widehat{C}_{\text{slope}}$  in Algorithm 2. On the one hand,  $\widehat{\sigma}_{m_0}^2$  estimates the asymptotic slope of  $-\|Y - \widehat{F}_m\|^2$  as a function of  $D_m$  from two points:  $m_0$  and  $m_1$  such that  $S_{m_1} = \mathbb{R}^n$ . On the other hand, Algorithm 2 makes a (robust) linear regression over, say, all  $m$  such that  $D_m \in [n/2, n]$ . An illustration is provided by Figure 10 in Appendix C. This confirms that minimal penalties—here, the slope heuristics—allow to avoid the choice of a single  $m_0 \in \mathcal{M}$  by making use of the full collection  $(S_m)_{m \in \mathcal{M}}$  for estimating the residual variance. Intuitively, this difference makes Algorithm 2 more stable and less dependent on some strong assumption about  $S_{m_0}$ . The numerical experiments of Figure 6b in Section 7.1 and Figure 10 in Appendix C indeed show that when  $S_{m_0}$  happens to be a bad model,  $\widehat{\sigma}_{m_0}^2$  can suffer from a large error, whereas  $\widehat{C}_{\text{thr}}$  is much more robust.

**Residuals of linear estimators** Residual-based estimators have also been proposed with several other linear estimators  $\widehat{F}_{m_0} = A_{m_0} Y$  of  $F$ , that is, defined as  $\widehat{\sigma}_B^2$  in Eq. (70) with a matrix  $B = (I_n - A_{m_0})^\top (I_n - A_{m_0})$ . For instance,  $A_{m_0}$  can correspond to some Nadaraya-Watson fit (also known as kernel-based estimator; Hall and Marron, 1990) or to spline smoothing (Carter and Eagleson, 1992); the article by Dette et al. (1998) provides more references. In the setting given by Eq. (69), the challenging case  $d > 1$  can be tackled with  $k$ -nearest neighbors (Litiäinen et al., 2010) or a local linear fit of  $f$  (Spokoiny, 2002). All these estimators suffer from the same drawback as  $\widehat{\sigma}_{m_0}^2$ , that is, they rely on the choice of a *single* matrix  $A_{m_0}$ , hence requiring to specify the regularization parameter  $m_0$ . On the contrary, the minimal-penalty approach of Algorithm 4 avoids this choice in a principled way.

**Difference-based estimators** Difference-based estimators are an important family of residual-variance estimators, which are designed for the setting of Eq. (69) when  $\|x_i - x_{i+1}\| = o(1)$  and  $f$  is smooth, often assuming  $d = 1$ . The first example has been proposed by Rice (1984),

$$\widehat{\sigma}_{\text{Rice}}^2 := \frac{1}{2(n-1)} \sum_{i=1}^{n-1} (Y_{i+1} - Y_i)^2,$$



which is close to the residual-based estimator defined by Eq. (74). More generally, difference-sequence estimators of order  $m \geq 1$  are defined by

$$\widehat{\sigma}_{(d_0, \dots, d_m)}^2 = \frac{1}{n-m} \sum_{i=1}^{n-m} \left( \sum_{j=0}^m d_j Y_{i+j} \right)^2 \quad \text{where} \quad \sum_{j=0}^m d_j = 0 \quad \text{and} \quad \sum_{j=0}^m d_j^2 = 1.$$

The only admissible sequence  $(d_j)_{j=0,1}$  for  $m = 1$  leads to  $\widehat{\sigma}_{\text{Rice}}^2$ . For a general order  $m$ , when  $x_i \in \mathbb{R}$ , the optimal sequence  $(d_j)_{j=0, \dots, m}$  in terms of MSE does not depend on  $f$  asymptotically and can be computed explicitly (Hall et al., 1990), although the picture can be quite different in a non-asymptotic setting (Dette et al., 1998).

Assuming  $x_i \in \mathbb{R}$ , difference-based estimators of order  $m \geq 1$  are suboptimal by a constant factor  $1 + 1/(2m)$  in terms of MSE for normal data (Hall et al., 1990), while for instance the residual-based estimator of Hall and Marron (1990) attains the optimal rate  $\text{var}(\varepsilon_1^2)/n$ . This issue is corrected for instance with covariate matching (Müller et al., 2003; Du and Schick, 2009), which in the case of order  $m = 1$  consists in replacing  $\widehat{\sigma}_{\text{Rice}}^2$  by

$$\frac{1}{2n(n-1)} \sum_{i \neq j} W_{i,j} (Y_i - Y_j)^2$$

with some well-chosen weights  $W_{i,j} \geq 0$  (Müller et al., 2003). Another variant of difference-based estimators, which is asymptotically optimal, is studied by Tong et al. (2013).

Choosing  $m$  and the sequence  $(d_j)_{j=0, \dots, m}$  is also a difficult problem with no prior knowledge (Dette et al., 1998). But the main drawback of such estimators is that, when  $f$  is not continuous, they can be severely biased in an unpredictable way. An empirical method for detecting whether the bias is small enough is proposed by Buckley and Eagleson (1989) and might be useful.

## 6.2. Estimation of the residual covariance matrix

Assume now that several regression problems such as (1) must be solved simultaneously, a framework known as “multi-task regression”, “multivariate regression”, “multiple linear regression”, and “seemingly unrelated regression”; the article by Solnon et al. (2012) and the PhD dissertation of Solnon (2013) provide references on this topic. One observes  $Y^j = F^j + \varepsilon^j \in \mathbb{R}^n$  for  $j = 1, \dots, p$ , assuming that the noise vectors  $\mathcal{E}_i := (\varepsilon_i^j)_{j=1, \dots, p} \in \mathbb{R}^p$  are independent and identically distributed, with zero mean and covariance matrix  $\Sigma \in \mathcal{M}_p(\mathbb{R})$ . Then, a natural extension of the residual-variance estimation problem is the estimation of  $\Sigma$  with as few prior knowledge on the  $F^j$  as possible, which is often required for the multi-task problem of estimating  $(F^j)_{j=1, \dots, p}$ . For instance, Solnon et al. (2012) make use of the prior knowledge that the  $F^j$  are close, in combination with kernel ridge regression, and selects regularization parameters with a penalty generalizing  $C_L$  which depends on the full matrix  $\Sigma$ .

An estimator  $\widehat{\Sigma}$  of  $\Sigma$  based upon minimal penalties is proposed by Solnon et al. (2012). It satisfies  $(1 - \eta)\Sigma \preceq \widehat{\Sigma} \preceq (1 + \eta)\Sigma$  with large probability, with  $\eta \propto p\sqrt{\log(n)/nc(\Sigma)^2}$  where  $c(\Sigma)$  is the condition number of  $\Sigma$ . The construction of  $\widehat{\Sigma}$  goes as follows:

- (i) For every  $j \in \{1, \dots, p\}$ , apply Algorithm 4 to the one-dimensional regression problem  $Y^j = F^j + \varepsilon^j$ , and store  $\widehat{a}_j = \widehat{C}_{\text{jump}}$  which estimates  $a_j := \Sigma_{j,j}$ .



- (ii) For every  $i \neq j \in \{1, \dots, p\}$ , apply Algorithm 4 to the one-dimensional regression problem  $(Y^i + Y^j) = (F^i + F^j) + (\varepsilon^i + \varepsilon^j)$ , and store  $\widehat{a}_{i,j} = \widehat{C}_{\text{jump}}$  which is an estimator of  $a_{i,j} := \Sigma_{i,i} + \Sigma_{j,j} + 2\Sigma_{i,j}$ .
- (iii) Denote by  $J$  the linear map on  $\mathbb{R}^{p(p+1)/2}$  that sends  $((a_j)_{1 \leq j \leq p}, (a_{i,j})_{1 \leq i \neq j \leq p})$  to  $\Sigma$ , and define  $\widehat{\Sigma} = J((\widehat{a}_j)_{1 \leq j \leq p}, (\widehat{a}_{i,j})_{1 \leq i \neq j \leq p})$ .

This construction can actually be generalized to any other one-dimensional residual-variance estimator  $\widehat{\sigma}^2$  that satisfies  $(1 - \eta_0)\sigma^2 \leq \widehat{\sigma}^2 \leq (1 + \eta_0)\sigma^2$  with large probability for all the above one-dimensional problems, leading to a similar result with  $\eta \propto c(\Sigma)p\eta_0$ . The remarkable property of the minimal-penalty-based estimator  $\widehat{\Sigma}$  of Solnon et al. (2012) is that it suffices to assume that an estimator of small complexity has a small approximation error —with slightly stronger constraints compared to Theorem 1, see the exact assumptions of Arlot and Bach (2011)— for each one-dimensional problem  $Y^j$  to get this assumption automatically satisfied for all the  $Y^i + Y^j$ ,  $i \neq j$ .

### 6.3. Model/estimator-selection procedures based on $C_p/C_L$

Let us go back to the model/estimator-selection problem in the fixed-design regression setting. For selecting among linear estimators with the least-squares risk, a popular penalization approach is Mallows'  $C_L$  (Mallows, 1973), as described in Section 3.3:

$$\widehat{m}_{C_L} \in \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \frac{1}{n} \left\| \widehat{F}_m - Y \right\|^2 + \operatorname{pen}_{C_L}(\sigma^2, m) \right\} \quad \text{with} \quad \operatorname{pen}_{C_L}(\sigma^2, m) := \frac{2\sigma^2 \operatorname{tr}(A_m)}{n}. \quad (78)$$

In the particular case of projection estimators,  $\operatorname{tr}(A_m) = D_m$  the dimension of the corresponding model, and  $C_L$  reduces to  $C_p$  which is described in Section 2.2. Both  $C_p$  and  $C_L$  penalties assume that the noise-level  $\sigma^2$  is known, so in general it must be replaced by some data-driven estimation of it. Minimal-penalty algorithms provide an estimator of  $\sigma^2$  specially built for this estimator-selection task (Algorithms 1 and 4), which can be plugged into Eq. (78) and for which theoretical guarantees can be proved, as shown by Theorem 1 and Arlot and Bach (2011). This subsection reviews some classical ways to estimate  $\sigma^2$  inside Eq. (78), as well as other estimator-selection procedures that are closely related, in the framework of Section 3.3 (linear estimator selection) and with its notation.

**Fixed variance estimator** A first option is to replace  $\sigma^2$  by some fixed estimator  $\widehat{\sigma}^2$  of this quantity, for instance chosen among the estimators described in Section 6.1. The most classical choice is to take a residual-based estimator  $\widehat{\sigma}_{m_0}^2$  as defined by Eq. (71), for some  $m_0 \in \mathcal{M}$  (Mallows, 1973; Efron, 1986; Baraud, 2000). For projection estimators, this option is often named “ $C_p$ ” and called “ $C_p(\mathcal{L}_0, \mathcal{L})$ ” by Efron (1986, Table 4). As discussed in Section 6.1, choosing  $m_0$  can then be as difficult as the original estimator-selection problem.

When using the penalty  $\operatorname{pen}_{C_L}(\widehat{\sigma}^2, m)$ , theoretical guarantees can be obtained if one can prove that  $\widehat{\sigma}^2$  is close to  $\sigma^2$  with large probability, in combination with Theorem 1 or its analogous for linear estimators. For instance, Baraud (2000, Theorem 6.1) does it for projection estimators with  $\widehat{\sigma}_{m_0}^2$  such that  $D_{m_0} = n/2$ ; the approximation error of  $m_0$  then appears as an additive term in the right-hand side of the oracle inequality.

Nevertheless, even if such guarantees imply some asymptotic-optimality result —provided that the approximation error of  $m_0$  tends to zero—, they might not help for choosing the best possible estimator  $\hat{\sigma}^2$  in terms of estimator selection, since these only are *upper bounds*. Indeed, the best bound is obtained when  $\hat{\sigma}^2$  is well concentrated around  $\sigma^2$ , but it is known that overpenalizing a bit —that is, taking  $\hat{\sigma}^2$  slightly larger than  $\sigma^2$ — empirically improves the estimator-selection performance (see Section 8.4). Residual-based estimators do overpenalize, because of the approximation error of  $m_0$ , but the overpenalization factor is unknown in practice and cannot be controlled without strong assumptions on the target  $F$ ; the consequences of a bad choice of  $m_0$  with  $\hat{\sigma}_{m_0}^2$  are illustrated in the numerical experiments of Section 7.1, see Figures 6–7.

On the contrary, minimal-penalty algorithms are more than a simple “plug in” of an estimator of  $\sigma^2$  —independent of the estimator-selection problem— inside  $\text{pen}_{C_L}$ . As detailed in Section 8.4, minimal-penalty algorithms seem to overpenalize slightly, by design, but a formal proof of this phenomenon remains an open problem.

**Variance estimator depending on  $m$**  Another approach is to plug into Eq. (78) a different variance estimator for each  $m \in \mathcal{M}$ , by considering the residuals on the model  $m$  for which the penalty is computed. In other words, assuming that  $D_m < n$  for all  $m \in \mathcal{M}$ ,  $\hat{m}$  is chosen by penalization with the penalty  $\text{pen}_{C_L}(\hat{\sigma}_m^2, m)$ . Let us consider projection estimators for simplicity. Then  $\hat{m}$  minimizes over  $m \in \mathcal{M}$  the criterion

$$\text{crit}_{\text{FPE}}(m) := \frac{1}{n} \left\| \hat{F}_m - Y \right\|^2 + \frac{2\hat{\sigma}_m^2 D_m}{n} = \frac{1}{n} \left\| \hat{F}_m - Y \right\|^2 \left( 1 + \frac{2D_m}{n - D_m} \right) \quad (79)$$

which has been proposed by Akaike (1969, 1970) under the name FPE —final prediction error— and is called “naive  $C_p$ ” or “ $C_p(\mathcal{L}_0, \mathcal{L}_0)$ ” by Efron (1986, Table 4). The FPE criterion (79) actually is a particular case of the multiplicative penalties defined by Eq. (59) in Section 4.6. More references and non-asymptotic oracle inequalities satisfied by such multiplicative penalties can be found in the article by Baraud et al. (2009), which explains in particular how the FPE criterion (79) should be enlarged, depending on the size of the collection  $\mathcal{M}$ . The main drawback of multiplicative penalties is probably that they need to deal carefully with the largest models. For instance, for FPE, the results of Baraud et al. (2009, Theorem 1) assume that for all  $m \in \mathcal{M}$ ,  $D_m \leq 0.39(n + 2) - 1$ , an assumption that can be weakened into  $D_m \leq \rho n$  for some  $\rho < 1$  when considering a modified multiplicative penalty (Baraud et al., 2009, Corollary 1).

**Generalized cross-validation** For choosing the regularization parameter of some smoothing methods, Wahba (1977) proposed the criterion called “generalized cross-validation” (GCV) defined as a rotationally invariant form of the cross-validation estimate, that is,

$$\text{crit}_{\text{GCV}}(m) := \frac{1}{n} \left\| \hat{F}_m - Y \right\|^2 \left( \frac{1}{n} \text{tr}(I_n - A_m) \right)^{-2}. \quad (80)$$

GCV can also be seen as a reweighted cross-validation estimate, which takes into account the asymmetry of the design (Craven and Wahba, 1978). Nevertheless, as remarked by Efron (1986, Remark W), “Despite its name, GCV is (nearly) a member of the  $C_p$  family of estimates”. Indeed, considering projection estimators only,

$$\text{crit}_{\text{GCV}}(m) = \frac{1}{n} \left\| \hat{F}_m - Y \right\|^2 \left( \frac{n}{n - D_m} \right)^2 \approx \frac{1}{n} \left\| \hat{F}_m - Y \right\|^2 \frac{n + D_m}{n - D_m} = \text{crit}_{\text{FPE}}(m) \quad (81)$$

where the approximation holds true when  $D_m \ll n$ . Theoretical guarantees for GCV are available in various settings (Li, 1985, 1987; Cao and Golubev, 2006), with the same limitation as the ones of FPE and other multiplicative penalties. For instance, Cao and Golubev (2006, Theorem 2) consider a truncated version of GCV where all  $m \in \mathcal{M}$  such that  $\text{tr}(A_m) > \sqrt{n}$  are discarded, and some examples exist where GCV is not asymptotically optimal (Li, 1986). Let us finally mention that an empirical comparison of GCV and minimal penalties (Algorithm 4) is done by Arlot and Bach (2009, 2011) for several kinds of linear estimators, showing that either Algorithm 4 clearly outperforms GCV or the two methods perform similarly, depending on the setting.

#### 6.4. L-curve, corner, and elbow heuristics

Minimal-penalty algorithms, in particular Algorithms 1–3, can be related to some “L-curve”, “corner” or “elbow” heuristics, which are often used for choosing hyperparameters in the statistics and machine-learning communities.

The L-curve is defined as a plot of the size of the residuals versus the size or the estimator complexity. Using the notation of Section 3, when the goal is to select an estimator among  $(\hat{s}_m)_{m \in \mathcal{M}}$ , the L-curve can be defined as  $(\mathcal{E}_m, \hat{\mathcal{R}}_n(\hat{s}_m))_{m \in \mathcal{M}}$ . For instance, the right part of Figure 2 in Section 2.4 shows an L-curve (the black dots); Figure 11 in Appendix C provides another illustration. The practical use of the L-curve has been suggested by Miller (1970) and Lawson and Hanson (1974, Chapters 25–26). Some precise heuristic choice of a regularization parameter—often called “the L-curve method”—has first been proposed by Hansen (1992) and Hansen and O’Leary (1993) for some inverse problem with Tikhonov regularization. The main idea is that the L-curve has three main parts:

- (i) a straight part where the residuals  $\hat{\mathcal{R}}_n(\hat{s}_m)$  decrease fastly while  $\mathcal{E}_m$  is almost constant, where the regularization is too strong,
- (ii) a flat part where  $\mathcal{E}_m$  increases much while the residuals  $\hat{\mathcal{R}}_n(\hat{s}_m)$  decrease slowly, where some overfitting occurs, and
- (iii) in between, a “corner” or “elbow”, where the regularization parameter is of the correct order.

Therefore, the L-curve is L-shaped—hence its name, given by Hansen and O’Leary (1993)—and the L-curve method suggests to choose  $m$  corresponding to the corner of the “L”.

Several definitions of the corner can be proposed, as well as several measures of “size” and “complexity” can be considered when plotting the L-curve (Hansen and O’Leary, 1993). The most common choice is to define the corner as the location where the L-curve has a maximal curvature (Hansen and O’Leary, 1993)—hence the name “maximum-curvature criterion” (Grodzevich and Wolkowicz, 2009) often used for this heuristics—and to look at the L-curve in log-log scale (Hansen and O’Leary, 1993), although several variants exist (Regińska, 1996). Additional practical problems need also to be solved, especially when  $\mathcal{M}$  is discrete (how to define the curvature of a finite set of points?) and when some computational issues arise, for instance because computing every single point of the L-curve is expensive (Hansen and O’Leary, 1993; Castellanos et al., 2002; Hansen et al., 2007; Heng et al., 2010). Another option, proposed for a change-point detection problem (Lung-Yut-Fong et al., 2015), relies on performing two linear regressions on the L-curve in order to identify its parts (i) and (ii); it can therefore be directly related with the “slope” formulation of minimal-penalty algorithms.

Empirical or theoretical studies of L-curve algorithms are available mostly for inverse problems with Tikhonov regularization (Hansen, 1992), truncated SVD (Hansen and O’Leary, 1993; Reichel and Rodriguez, 2013), or conditional-gradient regularization (Castellanos et al., 2002), showing reasonably good empirical performance. Several of the papers mentioned in this subsection show that L-curve algorithms compare favorably to generalized cross-validation (GCV) on simulated examples; for instance, Hansen (1992) show some similarity between GCV and L-curve algorithms, and report a tendency of GCV to overregularize. Nevertheless, the L-curve method is proved to be not consistent in several families of realistic examples (Engl and Grever, 1994; Vogel, 1996; Hanke, 1996), when the noise tends to zero or when the sample size tends to infinity. According to Hanke (1996), the reason for this inconsistency is that the corner seems to correspond to the minimal level of regularization—the minimal penalty, with the words of the present survey—more than to the optimal level; hence choosing  $m$  at the corner leads to some overfitting.

The L-curve can also be used similarly in unsupervised learning for choosing the number of clusters, where it is defined as a plot of the within-cluster dispersion as a function of the number of clusters. Indeed, as written by Tibshirani et al. (2001), “Statistical folklore has it that the location of such an ‘elbow’ indicates the appropriate number of clusters”. Various methods actually use a similar idea (Tibshirani et al., 2001; Sugar and James, 2003; Matias and Miele, 2017), although they are not straightforward applications of the method of Hansen and O’Leary (1993). Remark that procedures choosing the number of clusters using the slope heuristics show good experimental results, according to Baudry (2009, Section 4.4), Maugis and Michel (2011a), Bontemps and Toussile (2013) and Baudry (2015).

**Comparison with minimal-penalty algorithms** Let us start with their common points. Both corner/elbow heuristics and minimal-penalty algorithms are based on the L-curve: directly in Algorithm 2, indirectly in Algorithm 1 since  $(D_{\hat{m}(C)})_{C \geq 0}$  can be seen as a reparametrization of the convex hull of the L-curve. Both rely on the idea of detecting a sharp variation of an observable quantity (the curvature / the selected dimension in  $D_{\hat{m}(C)}$ ) in some region of interest (the optimal value of regularization parameters / the minimal value of the constant in front of the penalty). For both methods, a visual check (of the presence of an elbow / a jump) is possible, and strongly encouraged (Hansen and O’Leary, 1993; Baudry et al., 2012). The strength of the connection between elbow heuristics and minimal penalties is emphasized in the following three works. For choosing the constant in front of the penalty for change-point detection, Lavielle (2005, Remark 2) suggests an algorithm close to (but slightly different from) the slope-heuristics algorithm of Lebarbier (2005), which can be formulated as a maximal-curvature criterion on the L-curve. For Hawkes-process estimation via model selection, when the model collection is large, Reynaud-Bouret and Schbath (2010) remark that the true model generally corresponds to a sharp angle of the L-curve, hence propose an algorithm between the slope and elbow heuristics, which consists in choosing  $\hat{m}(\hat{C})$  with  $\text{pen}(m) = \mathcal{E}_m$  and  $\hat{C}$  equal to the opposite of the slope of the segment joining the first and the last point of the L-curve. For choosing the bandwidth of a Gaussian kernel for quantile estimation with one-class support vector machines, Vert (2006, Section 6.2.2) points out an “elbow effect” and locates the elbow region with a “maximal jump” procedure similar to Algorithm 1.

Nevertheless, several important differences must be pointed out between the two approaches. First, the elbow heuristics tries to localize directly the optimal  $m$  whereas the slope heuristics localizes it in two steps: first, it estimates the minimal penalty, then, it uses an estimated optimal penalty for selecting some  $m$ . Second, the assumptions made on the shape of the L-curve are different. The L-curve must be *exactly* L-shaped for elbow heuristics, since otherwise the curvature can be large far from the “true” elbow. On the contrary, the slope heuristics assumes a linear behavior of the empirical risk as a function of  $D_m$  (or  $\mathcal{C}_m$ ) only for large models (Algorithms 2 and 6), and makes an even milder assumption with its jump formulation (Algorithms 1 and 5; see Theorem 1). Third, theoretical grounds are much stronger for the slope heuristics (with strong optimality results like Theorem 1 in several settings) than for the elbow heuristics which is even proved inconsistent in some realistic cases (Engl and Grever, 1994; Vogel, 1996; Hanke, 1996).

Overall, we consider the slope heuristics and its generalization (minimal penalties) as a simple and principled way to localize an elbow on the L-curve (when there is one), and to make use of it for optimal model/estimator selection. In particular, a natural answer to the problem of choosing the scale at which the L-curve should be considered on the  $x$ -axis is given by Section 3.6: it should be (the shape of) the minimal penalty.

### 6.5. Scree test and related methods

For choosing the number of factors in factor analysis, or the number of components in principal components analysis, some classical methods can be related to minimal-penalty and L-curve algorithms.

**Scree test** The most popular one —named the scree test— has been proposed by Cattell for factor analysis (Cattell, 1966; Cattell and Vogelmann, 1977). It is based upon the “scree plot”, that is, a plot of the eigenvalues versus their rank (in decreasing order), which can be seen as an L-curve for factor analysis. The key remark made by Cattell (1966) is that the scree plot ends with a linear part —a scree—, and that the beginning of the linear part corresponds to the “correct” number of factors. Overall, the scree test chooses a number of factors equal to the rank of the starting point of the linear part at the end of the scree plot.

This idea is close to the “slope” formulation of minimal-penalty algorithms (Algorithms 2 and 6). By analogy, we can say that the starting point of the linear part in the scree plot is a “minimal regularization level” —an upper bound on the number of factors that should be kept at the end. This fits well the goal of the initial paper by Cattell (1966), which is not to find the exact true number of factors —a quantity which might be impossible to define formally—, but only to keep a number of factors which explain 95% to 99% of the “substantive variance”. Nevertheless, the scree test seems to be often used for estimating the “true number of factors” itself (Jackson, 1993).

Similarly to minimal-penalty and L-curve algorithms, making use of the scree test requires to overcome practical issues: Cattell remarks that “even a test as simple as this requires the acquisition of *some* art in administering it” (Cattell, 1966). For instance, it seems important to normalize the data (Cattell, 1966), and sometimes the scree plot ends with two or three linear parts —then, one should cut at the beginning of the first linear part (Cattell, 1966).

**Variants** Several variants of the scree test exist. The number of factors can for instance be given by the intersection of the scree plot with some reference curve, which corresponds to some “average scree plot” obtained with “pure noise”, as proposed by [Horn \(1965\)](#) and [Horn and Engstrom \(1979\)](#), and by Frontier’s broken stick method ([Frontier, 1976](#)).

Another variant exists for estimating the intrinsic dimension of some data set, inside a classification procedure ([Bouveyron et al., 2015b](#)). Given a decreasing sequence of eigenvalues  $(\lambda_{(j)})_{1 \leq j \leq n}$ , the estimated intrinsic dimension is the smallest  $j$  such that  $\lambda_{(j)} - \lambda_{(j+1)} \leq T$  for some threshold  $T$ , which can be chosen by cross-validation in the article by [Bouveyron et al. \(2015b\)](#). The underlying assumption is that the scree plot is L-shaped, and that the point where the discrete derivative goes below  $T$  corresponds to the “elbow”, or to the beginning of the linear part.

**Results** All these methods are only validated by numerical experiments ([Cattell and Vogelmann, 1977](#)). For instance, for principal component analysis, [Jackson \(1993\)](#) concludes that the broken stick method is one of the two best methods for choosing the number of components. The scree test tends to overestimate by one the number of components according to [Jackson \(1993\)](#), which is consistent with our remark above that it corresponds to a “minimal regularization level” —not an optimal one.

Note however that some theoretical results are proved for the closely related problem of low-rank matrix recovery from noisy data by hard-thresholding of singular values. In an asymptotic framework, when the goal is to minimize the asymptotic mean squared error in some specific asymptotic regime, [Gavish and Donoho \(2014\)](#) show that the optimal hard threshold can be written  $\lambda_*(m/n)\sqrt{n}\sigma$  when the matrix to recover is of size  $m \times n$ . Interestingly, the “minimal threshold”, which corresponds to the largest singular value obtained from pure noise, is asymptotically equal to  $(1 + \sqrt{m/n})\sqrt{n}\sigma$ . In the framework of [Gavish and Donoho \(2014\)](#), the scree test would correspond to using the “minimal hard threshold”, and it seems indeed reasonable to use it for estimating the rank (the number of factors). On the contrary, when the goal is to minimize some quadratic error, the optimal threshold is a bit larger: [Gavish and Donoho \(2014, Figure 4\)](#) show that

$$\forall m \leq n, \quad \lambda_*\left(\frac{m}{n}\right) > 1 + \sqrt{\frac{m}{n}}.$$

### 6.6. Thresholding under the null

A related approach, for choosing the threshold  $\lambda$  of thresholding estimators, starts by considering the minimal value  $\hat{\lambda}_{\min}$  of the threshold such that the estimator is equal to zero. Under the null hypothesis —that is, when the true signal is zero—,  $\hat{\lambda}_{\min} = \hat{\lambda}_{\min}^{\text{null}}$  corresponds to the *minimal* thresholding level, and any good threshold must be larger than  $\hat{\lambda}_{\min}^{\text{null}}$ . For instance, in the setting of the previous paragraph —that is, singular-values hard thresholding—,  $\hat{\lambda}_{\min}^{\text{null}}$  is of order  $(1 + \sqrt{m/n})\sqrt{n}\sigma$ , and [Gavish and Donoho \(2014\)](#) provide an explicit formula for the optimal threshold, which can be written  $c(m/n)\hat{\lambda}_{\min}^{\text{null}}$  for some  $c(m/n) > 1$ .

In a general setting, [Giacobino et al. \(2017\)](#) define the quantile universal threshold (QUT)  $\lambda^{\text{QUT}}$  as the  $(1 - \alpha)$ -quantile of  $\hat{\lambda}_{\min}^{\text{null}}$  for some  $\alpha \in (0, 1)$ . It turns out that QUT corresponds



to the universal threshold proposed for wavelet thresholding (Donoho et al., 1995), and it can be used much more generally, beyond hard or soft thresholding. For instance, for choosing the regularization parameter  $\lambda$  of the Lasso and related procedures in high-dimensional regression, good performance can be obtained with  $\lambda = c\lambda^{\text{QUT}}$  for some  $c > 1$  (Giacobino et al., 2017, Section 4.2).

QUT and Algorithm 1 have common points: they both start by identifying a minimal value for the parameter of interest ( $\lambda$  or  $C$ ), then multiply it by a constant factor to get an optimal value of the parameter. Their main difference lies in the definition of the minimal parameter value: it is obtained from data under the null-hypothesis for QUT, hence requiring to know—or at least to approximate—the null-hypothesis distribution, while Algorithm 1 defines it directly from the data, whatever their distribution.

Note that Section 7.5 details a procedure by Rozenholc (2012), that is a variant of minimal-penalty algorithms for change-point detection, and can also be seen as a null-hypothesis based calibration procedure, hence similar to QUT.

### 6.7. Other model/estimator-selection procedures

Many other model/estimator-selection procedures exist and are studied. A detailed account on these is far beyond the scope of this survey. This subsection only mentions a few of them, that are of interest in relation with minimal-penalty algorithms.

**Unknown variance** First, in addition to the procedures based upon  $C_p$  and  $C_L$  that are listed in Section 6.3, some procedures are specially built for dealing with the problem of not knowing the noise variance in regression, which is also what minimal-penalty algorithms do in the regression case. For instance, Baraud (2011) provides an abstract general-purpose estimator-selection procedure, which leads to the model-selection procedure of Baraud et al. (2014) for Gaussian model selection with unknown variance. We refer to the article by Giraud et al. (2012) for a detailed survey on high-dimensional variable-selection methods when the variance is unknown.

**Cross-validation and resampling** An important family of general-purpose estimator-selection procedures is cross-validation (Arlot and Celisse, 2010), and more generally all resampling-based selection procedures—e.g., resampling-based penalties (see Arlot, 2009, and references therein). Comparing them to minimal-penalty algorithms is interesting at least in two distinct situations.

First, when Algorithm 5 works with  $\text{pen}_0$  and  $\text{pen}_1$  known but  $C^*$  is unknown—for instance, for linear estimators in regression with the least-squares risk—resampling-based procedures are natural competitors, that can be used either for choosing the constant in front of  $\text{pen}_1$ , or directly for the initial estimator-selection problem. Then, minimal-penalty algorithms have a clear advantage over resampling, because of their much smaller computational cost (see Section 7.2), while they have comparable or better statistical performance according to both theoretical and experimental results, as shown for instance by Arlot and Bach (2011).

Second, when Algorithm 5 works with some unknown  $\text{pen}_0$  and/or  $\text{pen}_1$ , an option mentioned in Remark 3 in Section 4.2 is to estimate them by resampling. Then, the computational cost of



Algorithm 5 is comparable to that of cross-validation and other resampling strategies applied to the initial estimator-selection problem. In such cases, the interest of using minimal penalties is the precise non-asymptotic calibration of the constant in front of the resampling-based penalty, which is not guaranteed when using the theoretical value for this constant, since it is often based upon asymptotic considerations. In addition, the conjecture detailed in Section 8.4 suggests another reason for combining resampling and minimal penalties in such frameworks.

## 7. Some practical remarks

This section discusses several practical questions about the use of minimal-penalty algorithms. A more detailed study of some of them can be found in the survey by Baudry et al. (2012).

### 7.1. Several definitions for $\widehat{C}$

The minimal-penalty estimator  $\widehat{C}$  of the constant that should be put in front of the penalty  $\text{pen}_1$  can be defined in several ways, which leads to the practical issue of choosing one among these definitions. Two main approaches are proposed in the previous sections.

**Jump approach** First,  $\widehat{C}$  can be defined as the position  $\widehat{C}_{\text{jump}}$  of “the unique large jump” of  $C \mapsto \mathcal{E}_{\widehat{m}_{\min}^{(0)}(C)}$ , as in Algorithms 1, 3, 4, and 5. Section 2.5 suggests two ways to formally define  $\widehat{C}_{\text{jump}}$ : choosing the maximal jump  $\widehat{C}_{\text{window}}(\eta)$  over a geometric window  $[C/(1+\eta), C(1+\eta)]$ , and choosing the value  $\widehat{C}_{\text{thr.}}(T_n)$  of  $C$  for which  $\mathcal{E}_{\widehat{m}_{\min}^{(0)}(C)}$  goes under some threshold  $T_n$ . Another natural option is to choose the position of the maximal jump

$$\widehat{C}_{\text{maxj.}} \in \operatorname{argmax}_{C \geq 0} \left\{ \mathcal{E}_{\widehat{m}_{\min}^{(0)}(C^-)} - \mathcal{E}_{\widehat{m}_{\min}^{(0)}(C^+)} \right\},$$

that is, taking  $\lim_{\eta \rightarrow 0} \widehat{C}_{\text{window}}(\eta)$ .

**Slope approach** Second,  $\widehat{C}$  can be defined as  $\widehat{C}_{\text{slope}}$ , the opposite of the estimated value of the slope of the empirical risk as a function of  $\text{pen}_0$ , as in Algorithms 2 and 6. This approach can be formalized in several ways, using ordinary or robust linear regression, either over a fixed range  $[p_{\min}, p_{\max}]$  of values of  $\text{pen}_0$ , or with the method  $\widehat{m}_{\text{CAPUSHE}}$  proposed by Baudry et al. (2012, Section 4.2), which is based upon a stability study of the selected estimator and depends on some parameter  $pct \in (0, 1]$ .

Note that  $\widehat{C}_{\text{window}}$ ,  $\widehat{C}_{\text{thr.}}$ , and  $\widehat{C}_{\text{slope}}$  all depend on some hyperparameter ( $\eta$ ,  $T_n$ ,  $p_{\min}$  and  $p_{\max}$ ,  $pct$ ). We refer to Appendix D.2 for more details on each definition of  $\widehat{C}$  considered in this section.

**Theoretical comparison** Let us first compare theoretically the various definitions of  $\widehat{C}$ . For  $\widehat{C}_{\text{jump}}$ , when there is a single large jump in

$$C \mapsto \mathcal{E}_{\widehat{m}_{\min}^{(0)}(C)},$$

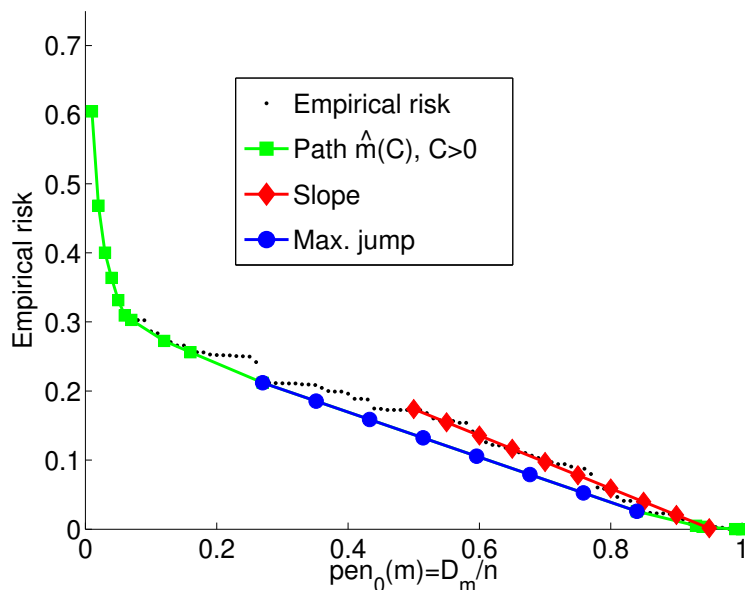


FIGURE 4. Connection between Algorithms 1 and 2: Plot of  $D_m \mapsto n^{-1} \|Y - \hat{F}_m\|^2$  and visualization of  $\hat{C}_{\text{slope}}$ . Setting called ‘easy’ in Appendix D.

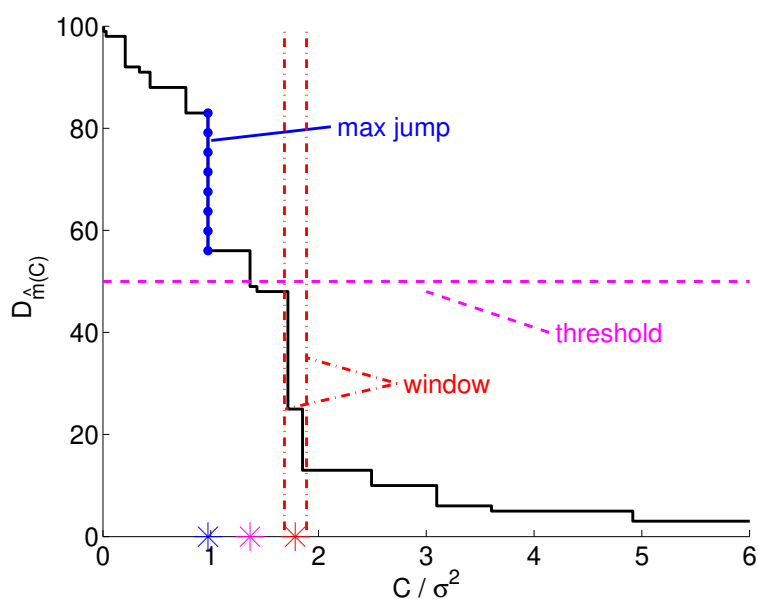


FIGURE 5. Plot of  $C \mapsto D_{\hat{m}(C)}$  (black solid lines) and visualization of the three versions of Algorithm 1 on the same sample. The maximal jump is shown by blue dots. The threshold value  $T_n = n/2$  is materialized by an horizontal dashed line. The largest jump over a window is shown by vertical dash-dot lines. The values of  $\hat{C}_{\text{max.j.}}$ ,  $\hat{C}_{\text{thr.}}$  and  $\hat{C}_{\text{window}}$  are shown by stars on the x-axis (in this order). The sample chosen here is not typical at all (see Table 1) but illustrates well the differences between  $\hat{C}_{\text{max.j.}}$ ,  $\hat{C}_{\text{window}}$  and  $\hat{C}_{\text{thr.}}$ . Setting called ‘easy’ in Appendix D.

as illustrated by Figure 2 in Section 2.4, reasonable choices for  $T_n$  and  $\eta$  make  $\widehat{C}_{\text{window}}(\eta)$  very close to  $\widehat{C}_{\text{maxj.}} = \widehat{C}_{\text{thr.}}(T_n)$ . On the contrary, when the phase transition around the minimal penalty yields several jumps of medium size in

$$C \mapsto \mathcal{E}_{\widehat{m}_{\min}^{(0)}(C)},$$

as in Figure 5 for instance,  $\widehat{C}_{\text{maxj.}}$ ,  $\widehat{C}_{\text{thr.}}(T_n)$ , and  $\widehat{C}_{\text{window}}(\eta)$  can take quite different values and lead to selecting different models. Theoretical guarantees such as Theorem 1 in Section 2.5 do not exclude such a situation, even asymptotically, so they only apply to  $\widehat{C}_{\text{thr.}}(T_n)$  and  $\widehat{C}_{\text{window}}(\eta)$  with  $T_n$  and  $\eta$  of the correct order of magnitude.

Yet, the maximal jump and threshold definitions with  $T_n = \overline{\mathcal{E}} := (\max_m \mathcal{E}_m + \min_m \mathcal{E}_m)/2$  coincide when the largest jump is of size at least  $(\max_m \mathcal{E}_m - \min_m \mathcal{E}_m)/2$ . This condition always holds true if no  $m \in \mathcal{M}$  has a complexity  $\mathcal{E}_m \in (\overline{\mathcal{E}}; \max_m \mathcal{E}_m)$ , which often occurs for computational reasons, since estimators with complexity  $\mathcal{E}_m > \overline{\mathcal{E}}$  usually are hard to compute and known to be suboptimal.

For the slope approach, no theoretical guarantee is available, but the linear behavior of  $\widehat{\mathcal{R}}_n(\widehat{s}_m)$  as a function of  $\text{pen}_0(m)$  is supported theoretically from expectation computations, as detailed in Sections 2.2–2.3 and 3.3–3.4.

The jump and slope approaches can seem quite different at first sight, but they actually are the two sides of the same coin. Section 2 shows that reasoning from the same computations, Eq. (7)–(8), can lead to a heuristic justification of both approaches. Another argument enlightens the similarity of the jump and slope approaches. By Proposition 5 and its proof in Appendix B.1, the path  $(\widehat{m}_{\min}^{(0)}(C))_{C>0}$  is piecewise constant,  $\widehat{m}_{\min}^{(0)}(C) = m_i$  for  $C \in [C_i, C_{i+1})$ , and the sequences  $(m_i)_{0 \leq i \leq i_{\max}}$  and  $(C_i)_{0 \leq i \leq i_{\max}}$  can be visualized on the L-curve  $(\text{pen}_0(m), \widehat{\mathcal{R}}_n(\widehat{s}_m))_{m \in \mathcal{M}}$ : the angles of the lower convex envelope of the L-curve exactly correspond to the  $m_i$ ,  $0 \leq i \leq i_{\max}$ , and

$$C_i = \frac{\widehat{\mathcal{R}}_n(\widehat{s}_{m_i}) - \widehat{\mathcal{R}}_n(\widehat{s}_{m_{i-1}})}{\text{pen}_0(m_{i-1}) - \text{pen}_0(m_i)}$$

is the opposite of the slope of the segment joining  $m_{i-1}$  to  $m_i$  on the L-curve. So,  $\widehat{C}_{\text{maxj.}}$  can be visualized on the L-curve, as illustrated by Figure 4. Given the L-curve (black dots), draw its (piecewise linear) lower convex envelope (green squares), localize the widest segment—in terms of values of  $\mathcal{E}_m$ , which is usually proportional to  $\text{pen}_0(m)$ —: its slope is  $-\widehat{C}_{\text{maxj.}}$ . Then, one clearly see why  $\widehat{C}_{\text{maxj.}}$  is often close to  $\widehat{C}_{\text{slope}}$  in the setting of Figure 4: for a random point cloud with a linear trend of slope  $\approx -C^*$  for large abscissa values, estimating its slope by linear regression is almost equivalent to looking at the slope of the longest segment of its lower convex envelope. Note that  $\widehat{C}_{\text{thr.}}$  can be visualized on the L-curve similarly to  $\widehat{C}_{\text{maxj.}}$ .

This direct comparison emphasizes the respective drawbacks of  $\widehat{C}_{\text{maxj.}}$  and  $\widehat{C}_{\text{slope}}$ . When the amplitude of the largest jump is small,  $\widehat{C}_{\text{maxj.}}$  is not a reliable estimation of  $C^*$ , see Figure 9b in Appendix C.

When some large models have a significantly positive approximation error, as in the ‘hard’ setting described in Appendix D—see the right of Figure 10—they pollute the slope estimation and make  $\widehat{C}_{\text{slope}}$  biased, unless only a few such models are present and robust regression is used. In the latter case, since  $\widehat{C}_{\text{jump}} \in \{\widehat{C}_{\text{maxj.}}, \widehat{C}_{\text{window}}, \widehat{C}_{\text{thr.}}\}$  only depends on the *lower convex envelope*

Configuration	All equal	Exactly 4 equal	At least 3 equal	All different	$\widehat{C}_{\max.j.} = \widehat{C}_{\text{thr.}}$	Max, thr, and win different
Frequency ('easy')	0.524	0.238	0.967	$< 10^{-3}$	0.777	0.009
Frequency ('hard')	0.134	0.118	0.894	$< 10^{-3}$	0.769	0.008

TABLE 1. Frequency of various configurations for the set of five models  $\widehat{m}$  respectively selected by Algorithm 1 with  $\widehat{C}_{\max.j.}$  ('max'),  $\widehat{C}_{\text{thr.}}$  ('thr'),  $\widehat{C}_{\text{window}}$  ('win'), by Algorithm 2 ( $\widehat{C}_{\text{slope}}$ ) and by  $\widehat{m}_{\text{CAPUSHE}}$ . 'Easy' and 'hard' settings, see Appendix D for details.

of the L-curve, even a large number of “polluting” models will not influence  $\widehat{C}_{\text{jump}}$  at all, making it more robust.

This difference between  $\widehat{C}_{\text{jump}}$  and  $\widehat{C}_{\text{slope}}$  also appears in the assumptions made for their theoretical and heuristic justifications. In Section 2,  $\widehat{C}_{\text{slope}}$  requires the approximation error to be almost constant over *all* large models—which makes sense when  $(S_m)_{m \in \mathcal{M}}$  is a family of models with increasing complexity, for instance, but can be violated in some other contexts—, whereas  $\widehat{C}_{\text{jump}}$  only assumes that *two* models exist with a small approximation error, one of moderate complexity and one of large complexity.

**Experimental comparison** In addition to the above theoretical comparison, we report the results of new simulation experiments for variable selection in least-squares regression. We consider two settings: in the ‘easy’ setting, the order between variables is known, while in the ‘hard’ setting, two possible orders (the correct one and its converse) are considered alternatively, making half of the models very bad. The ‘hard’ setting is the archetype of a setting where the approximation error is *not* constant over large models; it does not aim to be realistic. All details about simulation experiments—data generation, model collection, and exact implementation for each definition of  $\widehat{C}$ —are given in Appendix D.

First, since the beginning of this section outlines strong theoretical connections between the different definitions of  $\widehat{C}$ , a natural question is: how different are the models finally selected, depending on the definition taken for  $\widehat{C}$ ? Table 1 shows that they all coincide most of the time in the ‘easy’ setting—with a clear single large jump, as for the sample of Figures 2 and 4—and they globally agree at least 90% of the time or more in both settings. The probability of a total disagreement is very small (less than 0.1%) even if it sometimes occurs, as illustrated by Figure 5, where  $\widehat{C}_{\max.j.}$ ,  $\widehat{C}_{\text{thr.}}$ , and  $\widehat{C}_{\text{window}}$  respectively lead to selecting  $\widehat{m} = 14$ , 11, and 7; Figure 9b in Appendix C shows a similar configuration. Similar conclusions are obtained by Arlot and Massart (2009, Section 3.3) about  $\widehat{C}_{\max.j.}$  and  $\widehat{C}_{\text{thr.}}$ .

Second, since our experiments consider projection estimators in least-squares regression, all minimal-penalty based  $\widehat{C}$  estimate  $\sigma^2$ , so they can be compared to  $\widehat{\sigma}_{m_0}^2$ —defined by Eq. (71)—as estimators of the residual variance  $\sigma^2$ . Results are provided in Figure 6, as well as Tables 2–3 in Appendix C, where several values of parameters of the  $\widehat{C}$  are compared. In the ‘easy’ setting (Figure 6a), all methods behave similarly and as expected from theoretical arguments: the distribution of  $\widehat{C}$  is asymmetric around  $\sigma^2$ , with smaller deviations below  $\sigma^2$  than above  $\sigma^2$ , as in the bounds of Proposition 3. Such an asymmetry is a good property in terms of model-selection performance, as suggested by Figure 8 in Section 8.4 for instance. The order of magnitude of the deviations

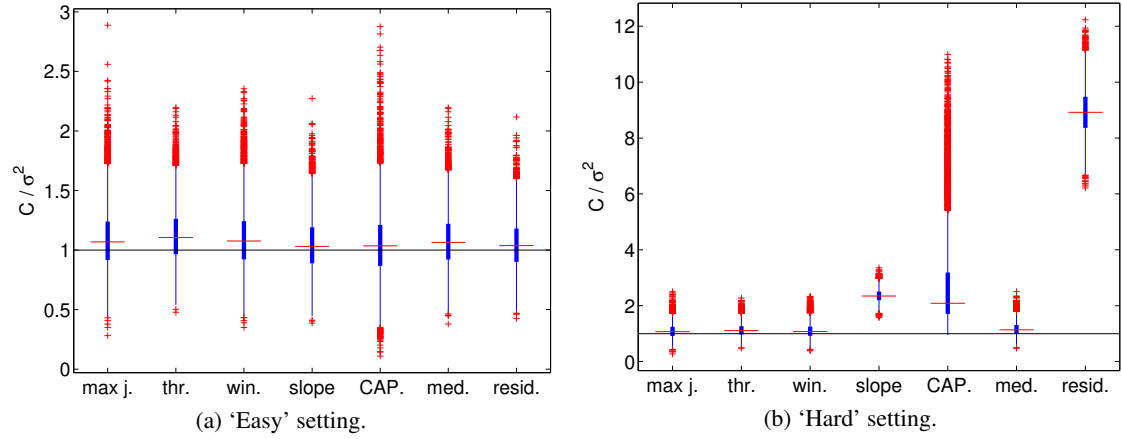


FIGURE 6. Distribution over 10000 independent samples of  $\widehat{C}/\sigma^2$  for seven estimators  $\widehat{C}$  of  $\sigma^2$ :  $\widehat{C}_{\max j.}$  ('max j.'),  $\widehat{C}_{\text{thr.}}$  ('thr. '),  $\widehat{C}_{\text{window}}$  ('win. '),  $\widehat{C}_{\text{slope}}$  in Algorithm 2 ('slope'),  $\widehat{C}_{\text{CAPUSHE}}$  ('CAP. '), the median of  $\{\widehat{C}_{\max j.}, \widehat{C}_{\text{thr.}}, \widehat{C}_{\text{window}}, \widehat{C}_{\text{slope}}, \widehat{C}_{\text{CAPUSHE}}\}$  ('med. '), and  $\widehat{\sigma}_{m_0}^2$  defined by Eq. (71) ('resid. '). See Appendix D for details.

of  $\widehat{C}_{\text{jump}}/\sigma^2$  from Proposition 3 is  $\mathcal{B}(c_n)/\sigma^2 + \sqrt{\log(n)/n}$  with  $c_n = n/3$  (for  $\widehat{C}_{\text{window}}$ ) or  $T_n/2$  (for  $\widehat{C}_{\text{thr.}}$ ); in our experiments, with  $n = 100$  and  $T_n = n/2$ , we get  $\mathcal{B}(c_n)/\sigma^2 \in [0.04, 0.08]$ , and  $\sqrt{\log(n)/n} \approx 0.2$ , so the constants appearing in Proposition 3 here are pessimistic.

The most variable  $\widehat{C}$  clearly is  $\widehat{C}_{\text{CAPUSHE}}$ , but to be completely fair, we must notice that the procedure proposed by Baudry et al. (2012) only outputs a selected model  $\widehat{m}_{\text{CAPUSHE}}$  and we make an arbitrary choice for defining some  $\widehat{C}_{\text{CAPUSHE}}$  from the definition of  $\widehat{m}_{\text{CAPUSHE}}$  (see Appendix D.2). Among other definitions of  $\widehat{C}$ ,  $\widehat{C}_{\max j.}$ , and  $\widehat{C}_{\text{window}}$  are slightly more variable than the others but the difference is mild.

Interesting differences occur in the 'hard' setting, which is designed as a case example for difficult situations for  $\widehat{C}_{\text{slope}}$ ,  $\widehat{C}_{\text{CAPUSHE}}$ , and  $\widehat{\sigma}_{m_0}^2$ . As expected,  $\widehat{C}_{\text{slope}}$  completely fails because of the wide amplitude of the approximation error among large models, and  $\widehat{\sigma}_{m_0}^2$  behaves totally differently depending on the parity of  $m_0$ :  $\widehat{\sigma}_{m_0}^2$  is worse than  $\widehat{C}_{\text{slope}}$  when  $S_{m_0}$  is one of the 'bad' models, while it works well when  $S_{m_0}$  is one of the 'good' models (see Figure 10 and Table 3 in Appendix C). This failure of  $\widehat{C}_{\text{slope}}$  and  $\widehat{C}_{\text{CAPUSHE}}$  —when  $(S_m)_{m \in \mathcal{M}}$  is the union of subcollections having different approximation properties— is also reported by Baudry (2009, Section 4.5), Devijver (2017b, Figures 3–4) and Devijver et al. (2019, Figure 6) in realistic settings. The nested algorithm presented in Section 7.3 might be a way to fix this issue, even if it has not been tested yet in such situations.

More generally, depending on the setting, choosing the parameter for one definition of  $\widehat{C}$  can be a big practical issue. For instance, Tables 2–3 in Appendix C show that  $\widehat{C}_{\text{thr.}}(T_n)$  is sensitive to the choice of  $T_n$ . Even if  $T_n = n/2$  works well for the 'easy' and 'hard' settings, it is certainly not a universally good choice, and changing  $F$ ,  $n$  or  $\sigma^2$  could easily make it fail compared to other definitions of  $\widehat{C}$ . Similarly, the performance of  $\widehat{C}_{\text{slope}}$  strongly depends on the parameters  $p_{\min}, p_{\max}$  and choosing them from data is not an easy task, a problem also reported in the change-point detection setting (Lebarbier, 2002, Chapter 4). A reasonable option is given by  $\widehat{m}_{\text{CAPUSHE}}$  (Baudry et al., 2012, Section 4.2), and it works reasonably well in the 'easy' setting, but it fails

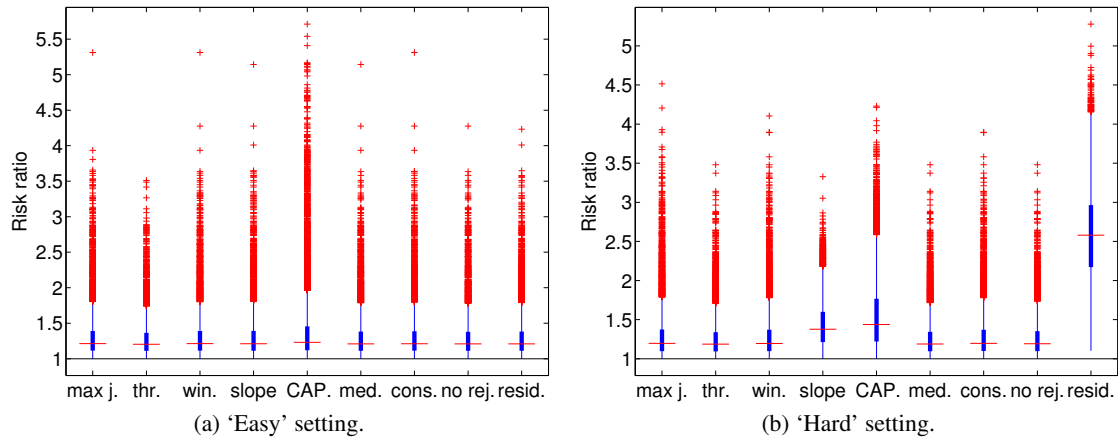


FIGURE 7. Distribution over 10000 independent samples of  $\|\widehat{F}_{\widehat{m}} - F\|^2 / \inf_{m \in \mathcal{M}} \|\widehat{F}_m - F\|^2$  for  $\widehat{m} = \widehat{m}(2\widehat{C})$  with  $\widehat{C}$  among the seven estimators  $\widehat{C}$  compared in Figure 6, and for  $\widehat{m}$  obtained by majority vote among  $\{\widehat{m}(2\widehat{C}_{\max.j.}), \widehat{m}(2\widehat{C}_{\text{thr.}}), \widehat{m}(2\widehat{C}_{\text{window}}), \widehat{m}(2\widehat{C}_{\text{slope}}), \widehat{m}_{\text{CAPUSHE}}\}$  with  $\widehat{m}(2\widehat{C}_{\text{window}})$  as a default choice ('cons.') or considering only the samples on which such a majority exists ('no rej.'). See Appendix D for details.

in the 'hard' setting as expected.

Third, the model-selection performance of all these procedures is assessed by Figure 7 and by Tables 2–3 in Appendix C.

At first order, the conclusions are similar to the ones obtained for estimating  $\sigma^2$ . All definitions of  $\widehat{C}$  work well in the 'easy' setting. In the 'hard' setting,  $\widehat{\sigma}_{m_0}^2$  completely fails, while  $\widehat{m}_{\text{CAPUSHE}}$  and  $\widehat{C}_{\text{slope}}$  do slightly worse than the other formulations of the slope-heuristics algorithm.

The detailed comparison of the procedures that work well is a bit different: the model-selection performance (risk ratios) are not ordered exactly as the mean-squared errors in Tables 2–3. The main reason is that risk estimation—which reduces to estimating  $\sigma^2$  in our setting—is different from model selection (Breiman and Spector, 1992). Figure 8 in Section 8.4 shows at least one reason for this difference: overpenalizing slightly, that is, overestimating  $\sigma^2$  a bit, improves the model-selection performance. According to Figure 8, the best overpenalization factor is 1.12 in the 'easy' setting. For instance, Table 2 shows that taking  $D_{m_0} = n/10$  for  $\widehat{\sigma}_{m_0}^2$  leads to better model-selection performance than  $D_0 = n/2$  in the 'easy' setting, even if  $D_0 = n/2$  yields a much better estimator of  $\sigma^2$ .

Note however that for a given bias (as an estimator of  $\sigma^2$ ), the best model-selection performance is obtained when the variance is the smallest: compare for instance  $\widehat{C}_{\text{slope}}$  with  $D_0 = n/2$  and CAPUSHE in the 'easy' setting (Table 2 in Appendix C).

Let us finally mention that previous simulation experiments in various settings have compared some of the definitions of  $\widehat{C}$ . In short, almost all of them report that  $\widehat{C}_{\max.j.}$  is less reliable—because of the event on which there is not a single large jump (Maugis, 2008, Figure 8.11; Baudry et al., 2012, Section 5), which happens more or less often—compared to  $\widehat{C}_{\text{thr.}}$  (Arlot and Bach, 2011; Solnon et al., 2012),  $\widehat{C}_{\text{window}}$  (Bontemps and Toussile, 2013), and  $\widehat{C}_{\text{slope}}$  or  $\widehat{C}_{\text{CAPUSHE}}$  (Baudry, 2009, Section 3.2; Maugis and Michel, 2011a; Connault, 2011; Baudry et al.,

2012; Roche, 2014, Table 2.1). Only Devijver and Gallopin (2018) report similar performances for  $\widehat{C}_{\max j.}$  and  $\widehat{C}_{\text{CAPUSHE}}$ . Nevertheless,  $\widehat{C}_{\max j.}$  remains useful for confirming the choice made with another definition of  $\widehat{C}$  (Connault, 2011; Baudry et al., 2012), with a visual check that there is a single large jump. The slope approach can also fail for reasons detailed previously in this subsection (Baudry, 2009; Devijver, 2017b; Devijver et al., 2019). Lebarbier (2005) even shows that  $\widehat{C}_{\max j.}$  and  $\widehat{C}_{\text{slope}}$  can both fail, which motivates a modified algorithm —called “calibrated method”— for change-point detection; note that Arlot et al. (2019) fix this precise failure by using the slope heuristics with a penalty shape depending on two constants, as detailed in Section 7.4.

**Conclusion on the choice of  $\widehat{C}$**  First, it is not surprising to have to choose among several definitions of  $\widehat{C}$  or to choose some hyperparameter such as  $\eta$ ,  $T_n$  or  $p_{\min}$ , because of no free lunch theorems: no fully automatic estimation procedure can work uniformly well over all statistical problems (Devroye et al., 1996, Chapter 7). An expert advice is always necessary at some point. For minimal-penalty algorithms, our suggests join the ones of Baudry et al. (2012) and Connault (2011): never use a single definition of  $\widehat{C}$  in a blind way, either by considering several definitions for  $\widehat{C}$  or by checking visually that there is a clear complexity jump and/or that the L-curve exhibits a clear linear trend on the data. When computing all values of  $(\widehat{\mathcal{R}}_n(\widehat{s}_m), \text{pen}_0(m), \text{pen}_1(m), \mathcal{C}_m)_{m \in \mathcal{M}}$  is too expensive, one should also take into account the computational cost of the procedure, as discussed in Section 7.2.

We propose the following (semi-automatic) approach for using several definitions  $\widehat{C}_{\max j.}$ ,  $\widehat{C}_{\text{thr.}}$ ,  $\widehat{C}_{\text{window}}$ ,  $\widehat{C}_{\text{slope}}$ , and  $\widehat{C}_{\text{CAPUSHE}}$  of  $\widehat{C}$  simultaneously. If the goal is to estimate  $\sigma^2$ , take their median. If the goal is estimator selection, compute the five corresponding estimator choices  $\widehat{m}$ , and make a majority vote: if at least three over five coincide, take their common value, otherwise, output a warning and ask the user to look at the complexity jump and the L-curve. When the five methods disagree, using a completely different approach remains a good option, for instance, cross-validation. The results of using this strategy (in a fully automatic way since our experiments need to be reproducible) are reported in Figures 6–7 above as well as Tables 2–3 in Appendix C, showing good performance in all settings.

Finally, the above comparison also points out several risky choices for  $\widehat{C}$  (in addition to  $\widehat{\sigma}_{m_0}^2$ ):  $\widehat{C}_{\max j.}$  without checking that there is indeed a single large jump,  $\widehat{C}_{\text{thr.}}$  with a bad choice for  $T_n$ , the “naive” version  $\widehat{C}_{\text{slope}}$  of the slope approach, and  $\widehat{C}_{\text{slope}}$  or  $\widehat{C}_{\text{CAPUSHE}}$  when selecting among a union of subcollection of estimators that may have different approximation properties.

## 7.2. Algorithmic cost

**When all empirical risks can be computed** Let us assume that the values of the empirical risk  $\widehat{\mathcal{R}}_n(\widehat{s}_m)$ , the minimal and optimal penalty shapes  $\text{pen}_0(m)$  and  $\text{pen}_1(m)$ , and the complexity  $\mathcal{C}_m$  for all  $m \in \mathcal{M}$  are stored in memory. Then, the computational complexity of minimal-penalty algorithms is the following.

For Algorithm 5, computing the full path  $(\widehat{m}_{\min}^{(0)}(C))_{C \geq 0}$  requires at most  $\mathcal{O}([\text{card. } \mathcal{M}]^2)$  operations —as shown in Appendix B.1— and much less in practice. Indeed, denoting by  $i_{\max} + 2$



the cardinality of this path —which must be smaller than  $\text{card}(\mathcal{M})$ —, it can be computed with  $\mathcal{O}(i_{\max} \text{card}(\mathcal{M}))$  operations.

Furthermore, depending on the definition of  $\widehat{C}_{\text{jump}}$ , it might not be necessary to compute the full path. For instance, with the threshold approach, using the notation of Appendix B.1, if  $i(T_n)$  is such that  $\widehat{C}_{\text{thr.}}(T_n) = C_{i(T_n)}$ , only  $\mathcal{O}(i(T_n) \text{card}(\mathcal{M}))$  operations are necessary, and usually we have  $i(T_n) \ll i_{\max} \ll \text{card}(\mathcal{M})$ .

Computing  $\widehat{C}_{\text{window}}$  as defined in Algorithm 5 might seem costly at first sight. Appendix B.2 shows that given the path  $(\widehat{m}_{\min}^{(0)}(C))_{C \geq 0}$ , of cardinality  $i_{\max} + 2$ , computing  $\widehat{C}_{\text{window}}$  can be done with at most  $\mathcal{O}(i_{\max} \log i_{\max})$  operations.

Finally, step 3 of Algorithm 5 requires at most  $\mathcal{O}(\text{card}(\mathcal{M}))$  operations. Overall, Algorithm 5 always has a complexity  $\mathcal{O}(i_{\max} \text{card}(\mathcal{M})) \leq \mathcal{O}([\text{card}(\mathcal{M})]^2)$ .

For Algorithm 6, step 1 is a (robust) linear regression —hence it has a computational cost  $\mathcal{O}(\text{card}(\mathcal{M}))$ — and step 2 can be done with  $\mathcal{O}(\text{card}(\mathcal{M}))$  operations. Note that  $\widehat{m}_{\text{CAPUSHE}}$  has a larger computational cost since it requires to run  $\mathcal{O}(\text{card}(\mathcal{M}))$  times Algorithm 6, hence a total cost of  $\mathcal{O}([\text{card}(\mathcal{M})]^2)$ .

**When computing all empirical risks is not tractable** In general, most of the computational complexity of computing  $\widehat{m}_{\text{Alg.5}}$  or  $\widehat{m}_{\text{Alg.6}}$  corresponds to computing  $\widehat{\mathcal{R}}_n(\widehat{s}_m)$  for all  $m \in \mathcal{M}$ . For instance, for density estimation with Gaussian mixture models (Maugis and Michel, 2011a), performing maximum-likelihood estimation in several large models involves a large computational cost, while we know that all corresponding estimators are always bad. Can we remove from the collection  $(\widehat{s}_m)_{m \in \mathcal{M}}$  most estimators with  $\mathcal{E}_m$  “large”, without degrading too much the performance of Algorithms 5–6?

For the jump approach, two estimators having a small approximation error are needed to get a jump, as with the assumptions of Theorem 1: one of large complexity, one much less complex. If we are not sure of which estimators have a small enough approximation error, considering more than two of them can be helpful; otherwise, this does not hurt —and we conjecture that this slightly decreases the variance of  $\widehat{C}_{\text{jump}}$ —, without being mandatory.

For the slope approach, the picture is different. Having only two estimators with a small approximation error implies making a linear regression over the corresponding two points, which is very close to the residual-based estimator  $\widehat{\sigma}_{m_0}^2$  defined by Eq. (71), as shown by Figure 10 in Appendix C. Therefore,  $\widehat{C}_{\text{slope}}$  with only a few large-complexity estimators faces the risk that some of them have a large approximation error, to which it will be quite sensitive, unlike  $\widehat{C}_{\text{jump}}$  (see Figure 10b). Using a robust regression in  $\widehat{C}_{\text{slope}}$  decreases the risk but does not exclude it totally, as shown by the poor results of  $\widehat{m}_{\text{CAPUSHE}}$  in our experiments in the ‘hard’ setting in Section 7.1.

A more reliable strategy for the slope approach —at least for settings a bit less difficult than our ‘hard’ setting— is to consider only estimators of complexity up to  $\mathcal{E}_{\max}$ , and to carefully check that  $\mathcal{E}_{\max}$  is large enough by visualizing the linear relation between the empirical risk and  $\text{pen}_0$ . This can be done easily with the CAPUSHE package (Baudry et al., 2012). The experiments of Baudry et al. (2012, Section 5) show as expected that  $\widehat{C}_{\text{slope}}$  is better —more stable— when  $\mathcal{E}_{\max}$  is large enough. Similarly, for change-point detection, Lebarbier (2002, Chapter 4; 2005, Section 4.2) studies the influence of such a bound  $\mathcal{E}_{\max}$  on  $\widehat{C}_{\text{max.j.}}$  and propose a heuristic method

—called “calibrated”— for choosing  $\mathcal{C}_{\max}$  from data.

Note finally that in some frameworks, well-chosen large-complexity estimators are easy to compute. For instance, in fixed-design regression, the estimator equal to the original data always has an empirical risk and an approximation error equal to zero —see assumption **(Hid)** in Theorem 1.

### 7.3. Nested minimal-penalty algorithm

In a framework where  $\mathcal{M}$  is a cartesian product  $\mathcal{M}_1 \times \mathcal{M}_2$ , [Devijver et al. \(2017\)](#) propose a “nested slope heuristics” algorithm, that we here generalize to Algorithms 5–6. The idea is to choose  $\hat{m} = (\hat{m}_1, \hat{m}_2) \in \mathcal{M}_1 \times \mathcal{M}_2$  in two steps. First, for every  $m_1 \in \mathcal{M}_1$ , select one estimator among  $(\hat{s}_{(m_1, m_2)})_{m_2 \in \mathcal{M}_2}$  with a minimal-penalty algorithm; the selected index is denoted by  $\hat{m}_2(m_1)$ . Then, select one estimator among  $(\hat{s}_{(m_1, \hat{m}_2(m_1))})_{m_1 \in \mathcal{M}_1}$  with a minimal-penalty algorithm. The numerical experiments of [Devijver et al. \(2017\)](#) on some transcriptomic data-analysis problem show that such a nested algorithm can work, for choosing a number  $m_1$  of clusters (of individuals) and a partitioning  $m_2$  of the features (the genes) used for inferring a cluster-dependent gene regulatory network.

### 7.4. Estimation of several unknown constants in the penalty

When the optimal penalty involves several unknown constants, that is,

$$\forall m \in \mathcal{M}, \quad \text{pen}_{\text{opt}}(m) = C_1^* \text{pen}_1^{(1)}(m) + \dots + C_k^* \text{pen}_1^{(k)}(m) \quad (82)$$

for some known  $\text{pen}_1^{(1)}, \dots, \text{pen}_1^{(k)}$ , the slope approach can be generalized, using linear regression for estimating simultaneously  $C_1^*, \dots, C_k^*$ . The idea has first been proposed with Algorithm 2 by [Lebarbier \(2002, Section 4.3.2\)](#) in the case of change-point detection, where the optimal penalty depends on  $k = 2$  constants.

It has since been used —with good numerical performance— in several settings: change-point detection ([Arlot et al., 2019](#)), joint variable selection and clustering via Gaussian mixture models ([Meynet and Maugis-Rabusseau, 2012](#)), principal curves estimation ([Biau and Fischer, 2012](#)), and unsupervised segmentation of spectral images via piecewise-constant Gaussian mixture models ([Cohen and Le Pennec, 2014](#)).

Nevertheless, no theoretical guarantees are currently available for such an algorithm. In addition to the practical issues already mentioned for the slope approach, this procedure is difficult to apply when there is not a single natural complexity measure  $\mathcal{C}_m$  but several of them — $\text{pen}_1^{(1)}(m), \dots, \text{pen}_1^{(k)}(m)$  can be  $k$  complexity measures—, which have to be combined wisely for defining what are the “complex enough”  $m \in \mathcal{M}$  over which the (robust) linear regression should be done. Another major difficulty is when  $\text{card}(\mathcal{M})$  or  $n$  are not large enough to allow a good estimation of several constants  $C_1^*, \dots, C_k^*$  simultaneously.

Another option is to make use of a simplified penalty shape —depending on a single multiplicative constant—, even when we know that it differs from the optimal shape given by Eq. (82).

Several articles make use of such a simplified penalty, instead of trying to calibrate  $k = 2$  constants, with satisfactory numerical results: for density estimation / clustering with Gaussian mixture models (Maugis and Michel, 2011a; see also Michel, 2008, App. C.2) or multinomial mixture models (Derman and Le Pennec, 2017), for choosing a simplicial complex in the computational geometry field (Caillerie and Michel, 2011), and for selecting jointly the rank and a set of variables in a high-dimensional finite mixture regression model (Devijver, 2017a).

A numerical comparison between simplified penalty shape and calibration of two constants is done in a few other papers, with various conclusions: favorable to the simplified shape (Lebarbier, 2002, Section 4.3.2, for change-point detection with Gaussian noise), similar for both methods (Devijver and Gallopin, 2018, for inference of a high-dimensional Gaussian graphical model), or favorable to the calibration of two constants —for change-point detection with Laplace noise and a simplified shape derived from experiments with Gaussian noise (Lebarbier, 2002, Section 4.6.4), for change-point detection with positive-definite kernels (Arlot et al., 2019), and for curve clustering (Meynet and Maugis-Rabusseau, 2012, Figure 5). As a conclusion, choosing between these two strategies should be done carefully, depending on the framework.

### 7.5. Variants for change-point detection

For change-point detection seen as a model-selection problem, three approaches closely related to minimal penalties have been proposed, without being exactly of the form of Algorithm 5. The first is the “calibrated method” (Lebarbier, 2005, Section 4.2) mentioned in Section 7.2.

Second, Lavielle (2005, Section 2.3) remarks that  $\hat{C}_{\max_j}$  often leads to underestimating the number of changes. Then, using the notation of Appendix B.1, it is proposed instead to define  $\hat{m}$  as the largest  $m_i = \hat{m}(C_i)$  corresponding to a jump whose height  $C_i - C_{i-1}$  is much larger than the one of the largest subsequent jump, that is,  $\max_{j>i}\{C_j - C_{j-1}\}$ . This approach might be closer to an elbow heuristics (see Section 6.4) than to a minimal-penalty algorithm.

**Statistical Base Jumping** Third, an unpublished idea by Rozenholc (2012) is the following. Assume that change-point detection is cast as a model-selection problem in fixed-design regression, so that we can use the notation of Section 2. Take some  $D$  “large” but, say, smaller than  $n/2$ , for instance  $D = n/\log(n)$  or  $D = \sqrt{n}$ . Compute  $\hat{F}_D$  the empirical risk minimizer over the set of piecewise-constant signals with  $D$  pieces (which is a union of  $\binom{n-1}{D-1}$  vector spaces of dimension  $D$ ). Consider the residual vector  $\tilde{Y} = Y - \hat{F}_D$  and apply the penalization approach to this pseudo-data, that is, compute

$$\forall C > 0, \quad \tilde{m}(C) \in \operatorname{argmin}_{m \in \mathcal{M}_n^{\text{chpt}}} \left\{ \frac{1}{n} \left\| \tilde{Y} - \Pi_m \tilde{Y} \right\|^2 + C \operatorname{pen}_0(m) + \operatorname{pen}'_0(m) \right\} \quad (83)$$

where the model collection  $\mathcal{M}_n^{\text{chpt}}$  is the one adapted to change-point detection, and the penalty shape  $C \operatorname{pen}_0(m) + \operatorname{pen}'_0(m)$  is a simplified version of the penalties proposed by Comte and Rozenholc (2004), Lavielle (2005) and Lebarbier (2005), such as

$$CD_m, \quad CD_m + \log \binom{n-1}{D_m-1} \quad \text{or} \quad C \log \binom{n-1}{D_m-1} + D_m.$$

Define  $\widehat{C}_{\text{SBJ}}$  as the minimal value of  $C > 0$  such that  $D_{\widehat{m}(C)} = 1$ , and finally select

$$\widehat{m}_{\text{SBJ}} \in \operatorname{argmin}_{m \in \mathcal{M}_n^{\text{chpt}}} \left\{ \frac{1}{n} \|Y - \Pi_m Y\|^2 + \frac{2\widehat{C}_{\text{SBJ}}}{1 + \frac{D}{n}} \operatorname{pen}_0(m) + \operatorname{pen}'_0(m) \right\}.$$

Note that  $\widehat{F}_D$ ,  $(\widehat{m}(C))_{C \geq 0}$  and  $\widehat{m}_{\text{SBJ}}$  can all be computed efficiently, in particular using dynamic programming. The heuristics behind this method is that if  $D$  is large enough to catch all true change-points of  $F$  in  $\widehat{F}_D$ , then  $\widetilde{Y}$  does not contain any signal anymore, and  $\widehat{C}_{\text{SBJ}} \operatorname{pen}_0$  is the minimal penalization level needed to recover with Eq. (83) the unique model of dimension one (constant signal). The factor  $1 + \frac{D}{n}$  dividing  $\widehat{C}_{\text{SBJ}}$  corrects for the variance of the pseudo-sample  $\widetilde{Y}$ . Unpublished experiments (Rozenholc, 2012) suggest that  $\widehat{m}_{\text{SBJ}}$  provides very good segmentations, much better than with the original slope heuristics—that is, Algorithm 1 or 2, as done by Lebarbier (2005) for instance.

### 7.6. Other uses of minimal penalties

Let us finish this section by mentioning two other uses of a minimal-penalty algorithm in the literature.

**Choice of a penalty shape** Algorithm 5 can be used for choosing among several penalty shapes, by detecting bad ones, which are the ones that do not lead to a clear dimension jump, as illustrated by Baudry et al. (2012, Section 3 of supplementary material) in the setting of Caillerie and Michel (2011).

**Minimal-penalty assisted experiments** For estimating a good deterministic constant  $\widetilde{C}^*$  to be put in front of the penalty, Chagny (2013) computes on 100 samples the constant  $\widehat{C}$  chosen by a slope heuristics algorithm, and defines  $\widetilde{C}^*$  as the maximal value of  $\widehat{C}$  observed over the 100 samples. The main interest of this approach is to require less computations than the standard one—which would be to compute, for every  $C$  in a grid, the average over the 100 samples of the risk of the estimator selected with the penalty  $C \operatorname{pen}_1$ , and then to take  $\widetilde{C}^*$  that minimizes the average risks over  $C$  in the grid—, even if the value  $\widetilde{C}^*$  might not be the optimal one.

## 8. Conclusion, conjectures, and open problems

As a conclusion of this survey, we sketch what is known theoretically for minimal-penalty algorithms, as well as several conjectures and open problems of high interest. Let us recall that Section 5 provides some hints for tackling many of these conjectures and open problems.

### 8.1. Settings and losses where minimal-penalty algorithms apply

Let us sketch the set of frameworks for which minimal-penalty algorithms are theoretically justified, at least partially (see Section 4).

The typical situation is a polynomial collection of minimum-contrast estimators (also called empirical risk minimizers) with a regular contrast (Saumard, 2010b) (for instance, the least-squares contrast), the corresponding risk (expected value of the contrast), and (almost) i.i.d. data.

Then, all obtained results show that  $\text{pen}_{\text{opt}} \approx 2 \text{pen}_{\text{min}}$ . In other terms, the slope heuristics holds true in several frameworks “close to” choosing among a polynomial collection of projection estimators with the least-squares risk and i.i.d. data.

The general result proved by [Saumard \(2010b, Chapters 7–8\)](#) for regular contrasts suggests that the slope heuristics is probably valid in all frameworks that are close enough to this ideal situation —e.g., least-squares estimators in regression or (conditional) density estimation with the least-squares risk—, under appropriate assumptions.

Two results, in regression ([Arlot and Bach, 2009](#)) and in density estimation ([Lerasle et al., 2016](#)), show that linear estimators can be considered instead of minimum-contrast estimators, at the price of changing the slope heuristics (Section 2) into a minimal-penalty heuristics (Section 3). A similar extension can probably be done in other settings for estimators that are (close to) linear functions of (part of) the data.

More generally, using the notation introduced in Section 4.1, it is probably often true that  $\mathbb{E}[p_2(m)]$  is a minimal penalty and  $\mathbb{E}[p_1(m) + p_2(m)]$  an optimal penalty. But unless these expectations are (approximately) known up to a multiplicative constant, applying such results requires to estimate  $\mathbb{E}[p_2(m)]$  and  $\mathbb{E}[p_1(m) + p_2(m)]$  by resampling (see Remark 3 in Section 4.2), and we then lose a nice feature of Algorithm 5 which is its small computational cost compared to cross-validation.

## 8.2. Unavoidable assumptions

Even in settings for which a full proof of a minimal-penalty algorithm is known, a natural question to ask is which assumptions are unavoidable for this algorithm to work.

Based upon existing proofs —in particular the one of Theorem 1, which is typical—, we conjecture that at least three assumptions are (almost) needed.

First, a “complex” estimator should be present in the collection, similarly to **(HId)**. Note that such an estimator can often be added on purpose to a predefined collection.

Second, one “less complex” but “good” estimator should also be present in the collection, similarly to what Theorem 1 assumes implicitly. The exact definition of “good” can depend on the context. In general, being consistent should suffice; note that assuming that the oracle estimator is consistent is a mild assumption for estimator selection, since otherwise the problem is not much interesting. In the setting of Theorem 1, it suffices to have a model with a small approximation error, even if the corresponding estimator is not consistent. Note however that such an assumption can be violated in practice, for instance when the estimator collection has not been well chosen, so that the approximation error never vanishes.

Third, it seems reasonable to make some mild moment assumption on the data so that the key quantities  $p_1$  and  $p_2$  concentrate around their expectations, at least when using deterministic penalty shapes. Nevertheless, a Gaussian assumption such as **(HG)** is not necessary ([Arlot and Massart, 2009](#); [Saumard, 2013](#)); see also Remark 1 in Section 2.5. Independence of data is not necessary either ([Lerasle, 2011](#); [Garivier and Lerasle, 2011](#)). Risk bounds could be obtained under much weaker moment assumptions —for instance, when the noise only has a finite moment of order two—, for empirical risk minimizers ([Mendelson, 2018](#)) or for robust estimators ([Audibert and Catoni, 2011](#), for instance). Nevertheless, we are not aware of any theoretical result

on minimal penalties in such a setting.

### 8.3. Other settings, losses, estimators

Numerical experiments show that minimal-penalty algorithms can be used fruitfully in many other settings such as supervised classification (Zwald, 2005), model-based clustering (Maugis and Michel, 2011a; Baudry, 2015), high-dimensional inference (Devijver and Gallopin, 2018), change-point detection (Lebarbier, 2005; Bardet et al., 2012), topological data analysis (Caillerie and Michel, 2011), functional linear models (Roche, 2014) or Hawkes-process intensity estimation (Reynaud-Bouret and Schbath, 2010), with applications in various domains such as biology —genomics (Akakpo, 2011; Reynaud-Bouret and Schbath, 2010), transcriptomics (Rau et al., 2015; Devijver and Gallopin, 2018), quantitative trait prediction from genomic data (Devijver et al., 2017), population genetics (Bontemps and Toussile, 2013)—, energy —electricity consumption prediction (Devijver et al., 2019), oil production modelization (Michel, 2008, Chapter 6)—, hyperspectral image segmentation (Cohen and Le Pennec, 2014), text analysis (Derman and Le Pennec, 2017), and bike sharing systems (Bouveyron et al., 2015a; Godichon-Baggioni et al., 2019). Combining these numerical experiments —especially the ones showing that the empirical risk is indeed close to a linear function of some known  $\text{pen}_0$  for large-complexity estimators— with the partial theoretical results available (Section 4), several settings can be identified where we conjecture that a minimal-penalty algorithm such as Algorithms 5–6 could be used fruitfully. Among them, we select below the most challenging ones, in terms of both practical applications and theoretical interest.

#### 8.3.1. Supervised classification

A classical setting where minimal-penalty algorithms would be quite useful is supervised classification with the 0–1 loss and corresponding empirical risk minimizers. No theoretical result is available up to now, and it seems tough to prove any because the 0–1 contrast is far from being regular. Nevertheless, Boucheron and Massart (2011) provide a key ingredient of the proof, that is, a concentration inequality for  $p_2(m)$  that applies easily to 0–1 classification, even when fast learning rates are possible. Given Proposition 1 and the general strategy detailed in Section 5, what remains is to prove a similar concentration inequality for  $p_1(m)$ , and to be able to estimate (up to the same unknown constant)  $\mathbb{E}[p_1(m)]$  and  $\mathbb{E}[p_2(m)]$ .

A probably easier open problem is to provide theory for the case of classification with a convex loss, such as the logistic loss —at the basis of logistic regression— or the hinge loss —at the basis of support vector machines. At least, for the hinge loss, the numerical experiments reported by Zwald (2005, Section 6.4.3) suggest that minimal-penalty algorithms can work with  $\text{pen}_0(m) = \mathcal{C}_m = D_m$  and  $\text{pen}_1(m) = 2D_m$ .

#### 8.3.2. Model-based clustering, choice of the number of clusters

Estimating the number of clusters for (unsupervised) clustering is another problem where fine tuning of penalties is a major challenge. A classical approach —called model-based clustering—



is to estimate the data density by maximum-likelihood on a mixture model, and to define clusters by a maximum a posteriori rule. Then, the number of clusters can be chosen by maximizing the penalized log-likelihood. Minimal-penalty algorithms with  $\text{pen}_0(m) = \mathcal{C}_m = D_m$  and  $\text{pen}_1(m) = 2D_m$  are shown successful by experiments on synthetic and real data, for various problems following this strategy (up to modifications that are specified below):

- clustering with Gaussian (Baudry, 2015), Poisson (Rau et al., 2015), multinomial (Derman and Le Pennec, 2017), or some functional (Bouveyron et al., 2015a) mixture models.
- clustering with Gaussian mixtures and the *conditional* log-likelihood instead of the log-likelihood, which leads to slightly different kinds of clusters (Baudry, 2015).
- joint clustering and variable selection—that is, identifying which features are relevant for clustering—with mixtures of Gaussian (Maugis and Michel, 2011a) or multinomial (Bontemps and Toussile, 2013) variables.
- efficient joint clustering and high-dimensional variable selection with maximum-likelihood estimators trained on *data-driven models* obtained by a first step of  $L^1$  penalization (Meynet and Maugis-Rabusseau, 2012); here, the shape of the minimal penalty seems to be close to a linear combination of  $D_m$  and  $D_m \log \frac{p}{D_m}$  (Meynet and Maugis-Rabusseau, 2012, Figure 6), and the algorithm described in Section 7.4 can be used.
- when an additional feature vector is provided for each observation, clustering a mixture of Gaussian regression models, jointly done with feature selection (Devijver, 2017b; Devijver et al., 2019) or partitioning (Devijver et al., 2017), via two-steps procedures similar to the one of Meynet and Maugis-Rabusseau (2012).

We conjecture that minimal-penalty algorithms indeed work in these settings, that is, as one can observe on synthetic or real data: (i)  $p_2(m)$  is (close to) a linear function of the number of parameters  $D_m$ , (ii) Algorithm 5 or 6 with  $\text{pen}_0(m) = D_m$  and  $\text{pen}_1(m) = \alpha D_m$  provides an estimator with a small Kullback-Leibler risk, for some  $\alpha > 1$  to be determined, and (iii) the number of clusters selected by this algorithm is equal to the true one  $K^*$  with large probability when  $n$  is large and the data distribution is close to a mixture with  $K^*$  components. Note that (ii) is a density estimation guarantee—hence, slightly different from clustering, but classical for justifying theoretically a penalty shape (Maugis and Michel, 2011b; Meynet and Maugis-Rabusseau, 2012; Bontemps and Toussile, 2013; Derman and Le Pennec, 2017; Devijver, 2017a)—and that (ii) and (iii) may require different values of  $\alpha$  since estimation and model identification are different goals for model selection, see Section 8.3.6. When variable selection is done jointly with clustering, (iii) can be completed by the fact that the true set of relevant variables is selected with large probability.

Up to now, only oracle inequalities with theoretical penalties are available in some of these settings. Of course, proving the above conjecture would be less difficult for pure model-based clustering (Baudry, 2015; Bouveyron et al., 2015a; Rau et al., 2015; Derman and Le Pennec, 2017) than for the two-steps algorithm using  $L^1$ -penalized maximum-likelihood for defining data-driven models (Meynet and Maugis-Rabusseau, 2012; Devijver, 2017b; Devijver et al., 2019).

Note also that variable selection, without any order among variables, means that the model collection considered is large—with the terminology of Section 4.7—, at least implicitly; this fact raises specific issues that are addressed in Section 8.3.4.



### 8.3.3. High-dimensional statistics

Hyperparameter tuning is a major issue for high-dimensional statistics (Giraud, 2014, Chapter 5), which can often be addressed by penalization. Despite several positive numerical results, providing a full theoretical proof of a minimal-penalty algorithm in this context remains an open problem.

**Clustering** Numerical results about minimal-penalty algorithms for joint (model-based) clustering and variable selection are reviewed in Section 8.3.2. For block-diagonal estimation of the covariance matrix of a high-dimensional Gaussian vector (graphical model), Devijver and Gallopin (2018) provide positive numerical results for a similar algorithm —maximum likelihood on data-driven models obtained by thresholding the empirical covariance matrix. Nevertheless, given the difficulty of proving an oracle inequality (Devijver and Gallopin, 2018, for instance), it seems hard to obtain a full theoretical validation of the minimal-penalty algorithms of Meynet and Maugis-Rabusseau (2012), Devijver (2017b) and Devijver and Gallopin (2018).

**Regression: the Lasso and related algorithms** One of the most classical high-dimensional statistics problem is variable selection in linear regression, for which the (group) Lasso and related algorithms are popular. Penalized least-squares can be used for choosing their parameters, thanks to covariance penalties (Efron, 2004), which have a simple expression of the form  $\sigma^2 df/n$  when the noise is Gaussian, where  $\sigma^2$  denotes the residual noise-level and  $df$  are the degrees of freedom. Easy-to-compute estimators of  $df$  exist for the Lasso (Tibshirani and Taylor, 2012; Dossal et al., 2013) and group Lasso (Vaiteer et al., 2012), among others. The remaining issue is to estimate  $\sigma^2$  without knowing any small correct model, for which minimal penalties are a natural approach (see Section 6.1).

The PhD dissertation of Connault (2011) provides an extensive numerical study of minimal penalties for calibrating either the Lasso or least-squares estimators trained on models selected by the Lasso (‘Lasso+LS’). In short, the major difficulty is that the natural candidate for  $\text{pen}_0(m)$ , that is  $\mathbb{E}[p_2(m)]/\sigma^2$ , cannot be used because it depends on the (unknown) signal  $\beta^*$ . Simplified penalty shapes —that is,  $\mathbb{E}[p_2(m)]/\sigma^2$  for a zero signal, or for a zero signal and an identity design matrix— often work for Lasso+LS, and sometimes for the Lasso, depending on the signal-to-noise ratio and on the sparsity of the signal. This is not satisfactory because these minimal-penalty algorithms sometimes fail for the Lasso or Lasso+LS, and Connault (2011) proposes “antidotes” for detecting the failure but nothing for correcting it, except using cross-validation.

It nevertheless seems possible to solve the case of an orthogonal design matrix, when the Lasso is soft thresholding and Lasso+LS is hard thresholding. Taking the number of selected variables  $k$  as tuning parameter, Loubes and Massart (2004, Section 2) conjecture that for soft thresholding,  $\mathbb{E}[p_2(k)] \approx \frac{3}{2} \frac{\sigma^2 k}{n}$ . If one could prove this conjecture, a minimal-penalty algorithm could be used for estimating  $\sigma^2$  —hence for calibrating soft (or hard) thresholding. Section 8.3.4 discusses the case of hard thresholding.

For a general design matrix and for other estimators, we think that the key question is to find the good parametrization of the estimator to be calibrated. For instance, the Lasso can be parametrized by the regularization parameter or by the number of selected variables, and Connault (2011) shows that the theoretical minimal penalty  $\mathbb{E}[p_2(m)]$  and the performance of

minimal-penalty algorithms strongly depend on the chosen parametrization. We also conjecture that the solution might not come from a direct application of Algorithms 5–6, but by the more general approach of identifying an observable phase transition —with respect to some well-chosen parameter— that provides the key information for an optimal calibration of the algorithm considered —for instance, an estimation of  $\sigma^2$  for the (group) Lasso. This idea has already been proposed in a few settings that are detailed in Section 8.5. For high-dimensional regression, theoretical results prove the existence of phase transitions in the risk of the Lasso (Bellec, 2017, Section 4; Bellec, 2018, Section 4.3) and of the constrained formulation of the Lasso (Chatterjee, 2014, Section 2.1). Nevertheless, it is not clear whether these phase transitions are observable, so they might not be useful for choosing hyperparameters. The approach of Section 6.6 seems to be another promising direction for tackling this problem.

Let us finally mention that concentration inequalities for  $p_1(m)$  are available for the Lasso and some related algorithms —see Section 5.3 for details. They can be useful for validating minimal-penalty algorithms.

#### 8.3.4. Large collection of models

As recalled in Section 4.7, the nature of the model-selection problem depends on the size of the model collection. All full proofs and almost all partial results available for minimal-penalty algorithms are for small collections, for which optimal model selection can be obtained with the unbiased risk estimation heuristics. For large collections, only a few partial theoretical results are available, as reported in Section 4.7. Therefore, the case of large collections remains a widely open problem of major interest.

The most classical situation is variable selection among  $p \gtrsim n$  variables, which amounts to select among a collection of  $2^p$  models. Let us start by focusing on the two settings where minimal-penalty algorithms are best understood: (i) variable selection with  $p = n$  and an orthonormal design —so that penalizing the least-squares criterion by a function of the number of variables is equivalent to hard thresholding—, and (ii) change-point detection —finding the locations of abrupt changes in the distribution of a sequence of  $n$  observations— which can be casted as a variable-selection problem with  $p = n - 1$  variables —the possible breakpoint locations— and solved by penalized least-squares.

Let us also recall that the notation  $(\beta)$ ,  $(\beta^-)$ ,  $(\beta^+)$ ,  $(\beta')$ ,  $(\gamma)$ , and  $(\tilde{\gamma})$  refer to partial results about minimal-penalty algorithms; they are defined in Sections 4.1–4.4.

**Orthonormal variable selection by hard thresholding** For variable selection with an orthonormal design and Gaussian noise, Birgé and Massart (2007, Proposition 2) prove  $(\beta')$  and  $(\tilde{\gamma})$  with a minimal penalty of order  $2\sigma^2 \frac{D_m}{n} \log \frac{n}{D_m}$  —at least for  $1 \ll D_m \ll n$ . We conjecture that  $(\beta)$  holds true in the same setting: a proof of  $(\beta^-)$  derives from the proof written by Birgé and Massart (2007, Proposition 2), and  $(\beta^+)$  seems easy to get given the results obtained by Birgé and Massart (2007). Then,  $(\beta)$  and  $(\tilde{\gamma})$  would prove that Algorithm 5, with  $\text{pen}_0(m) \approx D_m \log \frac{n}{D_m}$  and  $\text{pen}_1(m)$  given by Birgé and Massart (2007, Section 3.1.3), provides a good data-driven variable-selection procedure, satisfying an oracle inequality close to being optimal.

The main remaining challenge for having a full proof of a first-order optimal procedure is problem  $(\gamma)$ : find a first-order optimal penalty of the form  $\sigma^2 \text{pen}_1(m)$  with  $\text{pen}_1(m)$  known. We

think that this is a hard problem, whose resolution would have a great impact on model-selection theory in general, since even the *value* of the optimal excess risk of such a variable-selection procedure is not exactly known at first order. We only know by minimax arguments that it should be of order  $\log \frac{n}{D_m^*}$  times the oracle excess risk, up to a constant factor.

Another open problem for orthonormal variable selection is to determine the minimal penalty for non-Gaussian noise. Contrary to small model collections, this is not a straightforward extension of Gaussian results since the experiments of [Lebarbier \(2005, Section 5\)](#) for another large collection problem —change-point detection— suggest that the minimal penalty then is different for Laplace and for Gaussian noise.

**Change-point detection** Penalized least-squares is a classical approach to change-point detection, for which an oracle inequality ( $\tilde{\gamma}$ ) holds true for Gaussian noise and a penalty of the form  $\sigma^2 \frac{D_m}{n} [c_1 \log \frac{n}{D_m} + c_2]$  where  $c_1, c_2 > 0$  are two numerical constants and  $\sigma^2$  is the residual noise-level ([Lebarbier, 2005](#)); a similar result in a slightly different setting is proved by [Arlot et al. \(2019\)](#). The numerical experiments of [Lebarbier \(2005\)](#), [Sorba \(2017\)](#), [Garreau \(2017, Section 4.1\)](#), [Cabrieto et al. \(2018, Figure 4, for instance\)](#) and [Arlot et al. \(2019\)](#), as well as the partial theoretical results of [Sorba \(2017\)](#) —see Section 4.7—, suggest that a minimal-penalty algorithm with  $\mathcal{C}_m = D_m$  and  $\text{pen}_0(m)$  proportional to a linear combination of  $D_m$  and  $D_m \log \frac{n}{D_m}$  (or close to it, according to [Birgé and Massart, 2007](#), and [Sorba, 2017](#)) should work well in this setting. Given the numerical experiments of [Lebarbier \(2005\)](#) and [Arlot et al. \(2019\)](#), we conjecture that the ratio between the optimal and minimal penalty belongs to  $(1, 2]$ ; it may be model-dependent.

Proving these conjectures formally would require to solve two open problems: (a) prove the existence of a dimension jump for some known  $\text{pen}_0$  —or, equivalently, prove that step 2 of Algorithm 6, or its generalization of Section 7.4, works well—, and (b) prove an optimal oracle inequality for a penalty  $C^* \text{pen}_1$  that can be derived from the minimal penalty. Problem (b) is very hard, as for orthonormal variable selection. Problem (a) seems less difficult: [Sorba \(2017, Chapter 8\)](#) is close to proving it, but there is still a gap between “large enough” and “too small” penalties, which leaves open the possibility of having no clear dimension jump. It remains a challenge, as emphasized by the fact that the shape of the minimal penalty seems to depend on the noise distribution not only through its variance ([Lebarbier, 2005, Section 5](#)). Note that proving (a) with  $C^* = \sigma^2$  would be sufficient to get a good data-driven penalty for change-point detection, since an oracle inequality —maybe suboptimal— is already available for a penalty depending on  $\sigma^2$  and known quantities.

To conclude on change-point detection via penalized least-squares, let us recall that [Rozenholc \(2012\)](#) proposes a related but different approach to penalty tuning —see Section 7.5— that might be even more efficient than minimal-penalty algorithms for change-point detection with penalized least-squares. Justifying it theoretically would therefore be of great interest.

Beyond penalized least-squares, slope-heuristics algorithms empirically work well for change-point detection with dependent data in two settings: causal processes with the maximizer of a penalized log-likelihood ([Bardet et al., 2012](#)), and long-memory processes with the minimizer of a local Whittle contrast ([Bardet and Guenaizi, 2018](#)). [Bardet et al. \(2012\)](#) even show the remarkable fact that minimal penalties numerically adapt to variations of the optimal constant  $C^*$

—which can be of order  $\log(n)$  or  $\sqrt{n}$ — when the dependence structure varies. A theoretical validation of these results seems quite a challenge, since handling small model collections in the same settings already is an open problem.

**General setting** Understanding minimal-penalty algorithms for more general variable-selection problems seems a too high theoretical challenge for the next few years. We nevertheless conjecture that minimal-penalty algorithms work well beyond orthonormal variable selection and change-point detection, given the successful experiments of [Maugis and Michel \(2011a\)](#) and [Bontemps and Toussile \(2013\)](#) for joint variable selection and model-based clustering (see Section 8.3.2).

Minimal-penalty algorithms experimentally work well in several other settings mentioned previously, where large model collections are implicitly considered through  $L^1$  penalization or thresholding: model-based clustering ([Meynet and Maugis-Rabusseau, 2012](#)), multivariate regression with a mixture of linear models ([Devijver, 2017b](#); [Devijver et al., 2017](#)), and Gaussian graphical model estimation ([Devijver and Gallopin, 2018](#)).

### 8.3.5. Infinite estimator collections

Throughout the article, the estimator collection  $(\hat{s}_m)_{m \in \mathcal{M}}$  is assumed to be finite. Nevertheless, Algorithms 5–6 can still be used (at least theoretically, due to computational issues) for some infinite collections that behave as small (finite) collections, with the terminology of Sections 4.7 and 8.3.4.

Indeed, [Arlot and Bach \(2011\)](#) prove that Algorithm 5 can be used for selecting a tuning parameter within a *continuous set*  $\mathcal{M}$ . The proof of [Arlot and Bach \(2011\)](#) for kernel ridge regression mostly relies on two facts: (i) Algorithm 5 would work for a collection of  $L_1 n^{L_2}$  such estimators for any fixed  $L_1, L_2 > 0$ , (ii) the collection of kernel ridge regressors can be well approached by a finite collection of  $L_1 n^{L_2}$  estimators for some fixed  $L_1, L_2 > 0$ . We conjecture that a similar approach can be used for proving that Algorithm 5 works with some other continuous collections, starting by multiple-kernel ridge regression with a fixed number of kernels.

### 8.3.6. Model selection for identification of the true model

Throughout this survey, we assume that the goal is to choose a data-driven  $\hat{m} \in \mathcal{M}$  such that the risk of  $\hat{s}_{\hat{m}}$  is minimal, that is, satisfies a non-asymptotic oracle inequality (2). Model selection can target a different goal, which is to identify the smallest true model  $m^* \in \mathcal{M}$  with probability one asymptotically, assuming that some true model exists; a procedure  $\hat{m}$  achieving this goal is said “model-consistent”. Then, the exact same procedure cannot achieve the two goals in general ([Yang, 2005](#)). Can minimal-penalty algorithms still be useful for identification? Some experiments and theoretical arguments suggest a positive answer.

**Role of the size of the model collection** For large collections —see Section 8.3.4—, it turns out that both estimation and identification require to overpenalize compared to the unbiased risk estimation principle. Therefore, the minimal-penalty algorithms suggested in Section 8.3.4

should also work for identification. This conjecture is supported by the experiments of [Bontemps and Toussile \(2013, Figure 2\)](#) about variable selection in multinomial mixture models, and by those of [Arlot et al. \(2019, Figure 2\)](#) and [Garreau and Arlot \(2018, Figure 5–6\)](#) about change-point detection.

For small collections, the picture is different. A typical example is least-squares fixed-design regression with projection estimators, as in Section 2. Let us focus on this setting here for simplicity. The slope heuristics then leads to a model-selection procedure equivalent to  $C_p$ , which is first-order optimal for estimation but inconsistent for identification ([Shao, 1997, Theorem 1](#)). A simple way to fix this failure is to replace the factor 2 between minimal and optimal penalties in the slope heuristics by, say, a  $\log(n)$  factor, in order to get a BIC-type penalty, hence consistent for identification ([Shao, 1997, Theorem 2](#)). Such a correction of the slope heuristics may seem unsatisfactory, so one may consider to combine it with a procedure choosing from data between AIC and BIC-type penalties ([Yang, 2005; van Erven et al., 2012](#)).

**Change-point detection** For change-point detection with well-chosen small collections of models, [Gey and Lebarbier \(2008\)](#), [Durot et al. \(2009\)](#) and [Akakpo \(2011\)](#) propose specific hybrid procedures for identification of the change-point locations. In short, they consist of two-steps procedures, with minimal-penalty algorithms in both steps. The first step selects within a small model collection, providing an oversegmentation of the data sequence. The second step removes the unnecessary change-points. Proving the consistency of these procedures—including the minimal-penalty algorithms—is an open problem. Another natural question is to generalize such two-steps procedures to other model-selection problems with an identification goal.

**Minimal penalties for consistent identification** Let us finally mention some theoretical results about the minimal level of penalization needed for model consistency, that is, for having  $\hat{m} = m^*$  a.s. asymptotically. Even without a corresponding calibration algorithm—since the minimal penalty is not observable here—, this question remains of interest for theory.

In least-squares regression, [Shao \(1997, Theorem 1 \(iii\)\)](#) shows that  $C_p$  is not model consistent, assuming only that some true model  $m^* \in \mathcal{M}$  exists with  $D_{m^*} < D_{m^*} \leq D_{m^*} + \kappa$  for some fixed  $\kappa > 0$ . Such a result actually holds for any penalty of the form  $CD_m/n$  with  $C \geq 0$  fixed as  $n$  grows, which can be proved from arguments used in the proof of [Theorem 1](#). Conversely, using a penalty of the form  $\lambda_n D_m/n$  with  $\lambda_n \rightarrow +\infty$  and  $\lambda_n/n \rightarrow 0$  as  $n$  tends to infinity provides a model-consistent procedure ([Shao, 1997, Theorem 2](#)). Therefore, the minimal level of penalization for identification is of the form  $\lambda_n D_m/n$  with  $\lambda_n \rightarrow +\infty$ .

For maximum-likelihood estimators, at least two results are available. BIC-type penalties are minimal for estimating the order of a Markov chain without any prior upper bound on its order ([van Handel, 2011](#)). For density estimation with i.i.d. data, identifying the true model among a nested family by minimizing the log-likelihood penalized by  $\text{pen}(m) = f(m)g(n)$  requires that  $g(n) > C^*(s^*) \log \log n$  for some constant  $C^*(s^*) > 0$  ([Gassiat and Van Handel, 2013](#)).

### 8.3.7. Miscellaneous

**Model selection** Numerical experiments suggest that minimal-penalty algorithms work well for several other model-selection problems. We list them below, in order to help identifying settings where new theoretical results could be proved:



1. *Heteroscedastic regression* when the residual variance is known up to a constant —which can occur for inverse problems—, with least-squares risk and estimators (Villers, 2007, Section 2.6.2), beyond regressograms and strongly localized bases for which theoretical results are already known for a random design (Arlot and Massart, 2009; Navarro and Saumard, 2017). The fixed-design case can be handled similarly to the results of Arlot and Bach (2011). The random-design case with general models is clearly more challenging.
2. Estimation of two kinds of *geometrical objects*, with least-squares risk and estimators: simplicial complexes (Caillerie and Michel, 2011) and principal curves (Biau and Fischer, 2012).
3. *Least-squares risk and estimators* for clustering of compositional data (Godichon-Baggioni et al., 2019), Hawkes-process intensity estimation (Reynaud-Bouret and Schbath, 2010), and in a functional linear model (Roche, 2014, Section 2.4).
4. *Maximum-likelihood estimators with the Kullback-Leibler loss* for semiparametric regression with censored data via the Cox model (Letu , 2000), point-process intensity estimation (Michel, 2008, Section 6.3 and Appendix D.1.2), regression for counting processes under a proportional-hazard assumption (Oueslati and Lopez, 2013), and segmentation of spectral images via spatialized Gaussian mixtures (Cohen and Le Pennec, 2014).

**Estimator selection** We emphasize in this survey that minimal-penalty algorithms can be useful for estimator selection in general. Beyond the few theoretical results pointed out in Section 4.2, we conjecture that Algorithms 5–6 work for several estimator-selection problems.

First, numerical experiments suggest that they can be used for selecting among maximum-likelihood or least-squares estimators trained on *data-driven models*, obtained by  $L^1$  penalization in a variable-selection setting (Meynet and Maugis-Rabusseau, 2012; Devijver, 2017b), by thresholding the empirical covariance matrix (Devijver et al., 2017; Devijver and Gallopin, 2018), by  $k$ -means (Caillerie and Michel, 2011), or by (kernel) PCA in classification (Zwald, 2005, Section 6.4.3) or functional data analysis (Roche, 2014, Section 2.4). Some of these results are detailed above in Sections 8.3.2 and 8.3.3.

Second, minimal-penalty algorithms can be used successfully for the pruning step of CART in regression (Gey and Lebarbier, 2008) and of a spatial variant of CART (Bar-Hen et al., 2018), according to numerical experiments.

Finally, Algorithms 5–6 certainly cannot succeed for any kind of estimator collection. Section 8.5 describes a natural and promising way to generalize the minimal-penalty approach beyond Algorithms 5–6.

#### 8.4. Overpenalization

It is known empirically that a better model-selection performance can be obtained by overpenalizing a bit: the penalty  $C \text{pen}_{\text{opt}}^{\text{gal}}(m) = C \mathbb{E}[\mathcal{R}(\hat{s}_m) - \hat{\mathcal{R}}_n(\hat{s}_m)]$  has optimal performance when  $C$  is slightly above 1, as shown for instance by Arlot and Baudry (2002), Arlot (2007, Chapter 11) and Arlot (2009, Section 6.3.2) in the regression setting, and by Arlot and Lerasle (2016, Figure 3) in least-squares density estimation. A similar phenomenon holds in the experiments of Section 7.1, as shown by Figure 8. For histogram selection in density estimation, Saumard

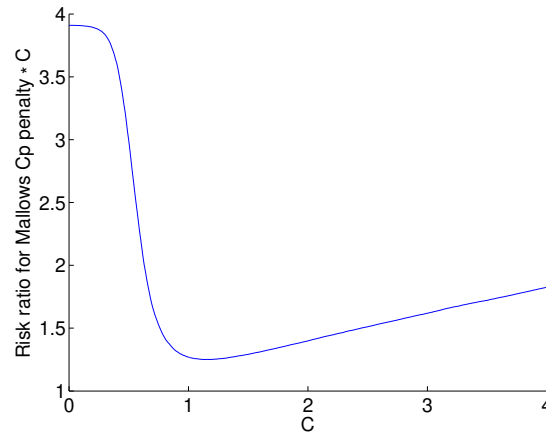


FIGURE 8. Overpenalization with Mallows'  $C_p$  penalty, 'easy' setting (see Appendix D.2 for details). Error bars are so small that they would not be visible on the graph. The optimal overpenalization factor is  $C = 1.12$ , leading to an improvement by a factor 1.015 compared to taking  $C = 1$ .

and Navarro (2018) propose a natural way to overpenalize automatically, which leads to a new corrected version of the AIC criterion. Nevertheless, choosing from data an appropriate overpenalization factor remains an open problem.

For reasons detailed below, we conjecture that minimal penalties can help solving this issue. More precisely, when Algorithms 5–6 are known to be first-order optimal, we conjecture that they automatically overpenalize —by a factor close to 1 when  $n$  is large—, and that this overpenalization decreases the risk of the final estimator compared to penalization by  $\text{pen}_{\text{opt}}^{\text{gal}}(m)$ . Another way to formulate this conjecture, following Lacour and Massart (2016) and Lacour et al. (2017, Section 2.4), is to state that the optimal constant  $C^*$  depends on  $n$  differently from what first-order asymptotics suggest, and that Algorithm 5 estimates well the finite-sample value of  $C^*$ . Section 2 certainly provides the less difficult setting for proving this conjecture, even if the challenge is high: it requires to analyze penalization procedures at a precision level an order of magnitude higher than ever.

Several results support the above conjecture. First, several simulation experiments show that minimal-penalty algorithms overpenalize slightly in most settings: this is reported by Villers (2007, Section 2.6.2.4), Arlot and Bach (2011) and Solnon et al. (2012, Section 6), and this holds for the experiments of Section 7.1 (see Figure 6 in Section 7.1 and Tables 2–3 in Appendix C).

Second, Theorem 1 is consistent with the fact that  $\hat{C}_{\text{jump}}$  might overestimate  $\sigma^2$ . Taking for instance  $T_n = n/2$ , Theorem 1 implies that on a large-probability event,

$$(1 - \eta_n^-) \sigma^2 \leq \hat{C}_{\text{thr.}}(T_n) \leq (1 + \eta_n^+) \sigma^2$$

with  $\eta_n^+ > \eta_n^-$ ; Proposition 3 in Section 6.1 provides a precise statement. If these bounds are tight, it means that  $\hat{C}_{\text{thr.}}$  is slightly biased upwards as an estimator of  $\sigma^2$ , which corresponds to overpenalization.

Third, minimal-penalty algorithms take into account the full collection of estimators  $(\hat{s}_m)_{m \in \mathcal{M}}$  in their definition, and Section 8.3.4 details why they should automatically adapt to the richness



of the collection  $\mathcal{M}$ . We claim that the need for overpenalization might be mostly related to the richness of  $\mathcal{M}$ , so that the conjectures of Section 8.3.4 could help solving the above overpenalization conjecture. Let us explain briefly why, by considering fixed-design regression with projection estimators, using some results and the vocabulary of Section 4.7. When  $\mathcal{M}$  is small—say, one model per value of the dimension—,  $\text{pen}_{C_p}(m) = 2\sigma^2 D_m/n$  is an (asymptotically) optimal penalty and the minimal penalty is  $\sigma^2 D_m/n$ . When  $\mathcal{M}$  is large—say,  $\binom{n}{D}$  models of dimension  $D$ —, the minimal amount of penalization required is multiplied by  $1 + 2\log(n/D_m)$ , which is of order  $2\log(n) \gg 1$  (except for the largest models), and good performance can be obtained with some penalties of the same order of magnitude. For a given sample size  $n$ , between these two extreme settings, there is a continuum of collections  $\mathcal{M}$  of increasing sizes, for which the optimal amount of penalization is  $C_n^*(\mathcal{M}) \text{pen}_{C_p}$  for some  $C_n^*(\mathcal{M})$  between 1 and  $2\log(n)$ , approximately: this is an instance of the overpenalization phenomenon. So, if a minimal-penalty algorithm adapts to the size of  $\mathcal{M}$ , it would capture the need for overpenalization by  $C_n^*(\mathcal{M})$  in the constant  $\widehat{C}_{\text{jump}}$ . At least,  $\widehat{C}_{\text{jump}}$  would be asymptotically of the correct order for both small and large  $\mathcal{M}$ , which cannot be done with some estimator  $\widehat{\sigma}^2$  that does not take into account the collection  $\mathcal{M}$ .

### 8.5. Beyond Algorithms 5–6: phase transitions for estimator selection

Most, if not all, nonparametric estimators depend on one or several parameters, whose optimal data-driven choice is often a challenge. In this survey, we focus on a single parameter  $C$  that is a multiplicative constant in front of a penalty, and we show that in several settings:

- (i) an observable phase transition occurs for the estimator  $\widehat{s}_{\widehat{m}_{\min}^{(0)}(C)}$  around  $C = C^*$ , and
- (ii)  $C^*$  can be used for the optimal calibration of  $\widehat{s}_{\widehat{m}_{\text{opt}}^{(1)}(C)}$  through Algorithm 5.

If a similar phenomenon occurs for other types of tuning parameters, this would lead to highly interesting generalizations of Algorithm 5. This subsection collects partial theoretical results—using the notation  $(\beta)$ ,  $(\beta')$ ,  $(\gamma)$  and  $(\widetilde{\gamma})$  defined in Sections 4.1–4.4—and experiments going into this direction, as well as several conjectures and open problems.

#### 8.5.1. Goldenshluger-Lepski's and related procedures

Goldenshluger-Lepski's method (Goldenshluger and Lepski, 2011; Bertin et al., 2016) is a classical estimator-selection procedure, which does not rely on penalization of an empirical risk but on pairwise comparisons between estimators.

**Goldenshluger-Lepski's method** For choosing the bandwidth  $h$  of kernel density estimators with a fixed kernel, in order to minimize the least-squares risk, Lacour and Massart (2016) study a slightly simplified version of Goldenshluger-Lepski's method, that depends on a single parameter  $a$  that can be interpreted as a constant in front of a penalty. If we define the complexity by  $\mathcal{C}_h = \|K\|^2/(nh)$ , as usual for kernel density estimation, Lacour and Massart (2016, Theorem 3) prove an equivalent of  $(\beta^-)$  and  $(\beta'^-)$  if  $a < 1$ , and  $(\widetilde{\gamma})$  if  $a > 1$ . Simulation experiments suggest that there is indeed a phase transition for the selected bandwidth around some value  $a^*$  of  $a$ —hence,  $(\beta^+)$  should also hold true—and that the optimal value of  $a$  is slightly above  $a^*$ .

Despite the theoretical results showing that  $a^* \rightarrow 1$  as  $n \rightarrow +\infty$ , for a finite sample size  $a^*$  is not necessarily close to 1. This leads to a minimal-penalty algorithm for estimating  $a^*$ , hence calibrating (a simplified version of) Goldenshluger-Lepski's method. The numerical experiments of two papers show the interest of this algorithm, with  $\hat{a}$  defined similarly to  $\hat{C}_{\max j.}$ : for estimating the stationary distribution of a bifurcating Markov chain on  $\mathbb{R}^d$  (Bitseki Penda and Roche, 2017), and for state-by-state inference of the emission densities of a hidden Markov model (Lehéricy, 2018). Although Lehéricy (2018) takes a penalty multiplied by  $a = 2\hat{a}$  for defining the final estimator—similarly to the slope heuristics—, Bitseki Penda and Roche (2017) take  $a$  just above  $\hat{a}$ , by selecting the estimator immediately after the jump of  $\mathcal{C}_h$ . This choice is supported by the fact that the minimal and optimal penalties are almost equal in the results of Lacour and Massart (2016).

**Penalized comparison to overfitting (PCO)** In the same framework, with a possibly multivariate bandwidth  $h \in \mathbb{R}^d$ , Lacour et al. (2017) propose a new procedure called penalized comparison to overfitting (PCO), which lies between penalization and Goldenshluger-Lepski's method. PCO depends on a parameter  $\lambda$  which is a multiplicative factor in front of one of the two terms of some kind of penalty. Considering again the complexity  $\mathcal{C}_h = \|K\|^2/(nh)$ , PCO satisfies an equivalent of  $(\beta^-)$  if  $\lambda < 0$  (Lacour et al., 2017, Theorems 3–4),  $(\beta^{'+})$  if  $\lambda > 0$ , and  $(\gamma)$  around  $\lambda = \lambda^* = 1$  (Lacour et al., 2017, Theorems 2 and 5). The optimality of  $\lambda^* = 1$  is assessed by numerical experiments on synthetic data (Varet et al., 2019).

Although PCO does not seem to require a data-driven calibration of  $\lambda$  according to the above result,  $\lambda = 1$  may not always be a good choice outside the least-squares density estimation setting. Therefore, the theoretical results of Lacour et al. (2017) suggest the following minimal-penalty algorithm for calibrating PCO: first, detect  $\hat{\lambda}$  around which  $\lambda \mapsto \mathcal{C}_{h(\lambda)}$  jumps, then, take

$$(a) \quad \lambda = \hat{\lambda} + 1 \quad \text{or} \quad (b) \quad \lambda = 2(\hat{\lambda} + 1) - 1 = 2\hat{\lambda} + 1$$

for defining the final estimator. Option (a) is suggested by the fact that the difference between the minimal  $\lambda$ —zero— and the optimal  $\lambda$ —one— is equal to 1 (Varet et al., 2019, Remark 3.1). Option (b) is suggested by the slope heuristics, since the penalty  $\lambda \text{pen}_0$  is equivalent to  $C \text{pen}_0 - \text{pen}_0$  with  $C = \lambda + 1$ , for which the minimal penalty occurs at  $C = 1$  and the (asymptotically) optimal penalty occurs for  $C = 2$ —hence a factor 2 between the minimal and the optimal penalty.

The experiments of Comte et al. (2017, Section 5) suggest that a similar way to calibrate PCO works well for selecting the bandwidth of a kernel estimator of the stationary density of the solution of a stochastic differential equation. For state-by-state inference of the emission densities of a hidden Markov model, Lehéricy (2018, Section 4.3.2) proposes a variant of PCO that can be well calibrated by a minimal-penalty algorithm according to numerical experiments.

A full theoretical validation of this calibration strategy remains an open problem. Providing theoretical guidelines for choosing between options (a) and (b) would also be interesting. Another natural question is to generalize PCO to other settings where Goldenshluger-Lepski's method applies, such as density estimation with the  $L^p$  risk or regression; to the best of our knowledge, this remains an open problem.

### 8.5.2. Choice of a threshold

For some thresholding estimators, with a threshold depending (non-linearly) on some parameter  $\gamma \in (0, +\infty)$ , an equivalent of  $(\beta')$  is proved—for a particular basis and assuming that  $s^*$  is equal to  $\mathbb{1}_{[0,1]}$ —, as well as an equivalent of  $(\tilde{\gamma})$  in the general case, in two settings: density estimation on  $\mathbb{R}$  (Reynaud-Bouret et al., 2011) and estimation of a Poisson intensity on  $\mathbb{R}$  (Reynaud-Bouret and Rivoirard, 2010).

For some Dantzig estimator (given some dictionary), with a parameter  $\gamma > 0$  appearing in the Dantzig constraints, Bertin et al. (2011) prove an equivalent of  $(\beta')$ —for a particular dictionary and assuming that  $s^* = \mathbb{1}_{[0,1]}$ —, as well as an equivalent of  $(\tilde{\gamma})$  in the general case.

In all the above results (Reynaud-Bouret and Rivoirard, 2010; Bertin et al., 2011; Reynaud-Bouret et al., 2011), an equivalent of Algorithm 5 is proposed for a data-driven choice of  $\gamma$ , and numerical experiments suggest that the optimal  $\gamma$  is often very close to the minimal  $\gamma$ . Therefore, a generalization of the slope heuristics ( $\gamma_{\text{opt}} \approx 2\gamma_{\text{min}}$ ) probably does not hold here.

### 8.5.3. Generalization

The above results, obtained for two different kinds of problems, suggest that phase transitions could be used much more generally for estimator selection, including the optimal calibration of learning algorithms. Section 8.3.3 proposes it for the Lasso and related procedures. We conjecture that the same idea can be used fruitfully in several other settings.

The key question is to find the good parametrization of the estimator collection. The successes of minimal-penalty algorithms rely on the parametrization by the constant  $C$  in front of a well-chosen penalty shape  $\text{pen}_0$ —that is, chosen following the theoretical guidelines of Section 5.1, possibly combined with the practical hints referenced in Section 7.6.

Finding an appropriate parametrization for the Lasso, for instance, remains an open problem to the best of our knowledge.

## 8.6. Related challenges in probability theory

Addressing the statistical open problems listed above mostly relies on a few corresponding open problems in probability theory. As detailed in Section 5, for each estimator  $\hat{s}_m$  considered, given some deterministic  $s_m^*$ —which can be the best estimator in the associated model, or the expectation of  $\hat{s}_m$ , for instance—, the key theoretical quantities are the following:

- the excess risk  $p_1(m) = \mathcal{R}(\hat{s}_m) - \mathcal{R}(s_m^*)$ ,
- the excess empirical risk  $p_2(m) = \hat{\mathcal{R}}_n(s_m^*) - \hat{\mathcal{R}}_n(\hat{s}_m)$ ,
- the empirical process at  $s_m^*$ ,  $\delta(m) = \mathcal{R}(s_m^*) - \hat{\mathcal{R}}_n(s_m^*)$ .

Since the empirical process is well understood in general, the main challenges are about  $p_1(m)$  and  $p_2(m)$ . One either has to show that  $|p_1(m) - p_2(m)|/p_1(m)$  is small on a large-probability event—using Proposition 2 in Section 5.2.2—, or to show non-asymptotic concentration inequalities for  $p_1(m)$  and  $p_2(m)$  around deterministic quantities that are known up to a multiplicative factor.

We strongly encourage further work on these questions, especially on the concentration of the excess risk  $p_1(m)$  and the excess empirical risk  $p_2(m)$ , which are difficult theoretical problems

of interest for statisticians beyond minimal penalties.

Indeed, concentrating the excess risk provides lower bounds on the risk of the estimator  $\hat{s}_m$  for a given statistical problem—and not in the minimax sense, as most statistical lower bounds—, which can be much informative for practitioners. This problem has attracted some attention in the last few years, and we review the recent work on this topic in Section 5.3.

When  $\hat{s}_m$  is the empirical risk minimizer over some model  $S_m$ , the excess empirical risk can be rewritten as the supremum of an empirical process

$$p_2(m) = \sup_{t \in S_m} \{ \widehat{\mathcal{R}}_n(s_m^*) - \widehat{\mathcal{R}}_n(t) \},$$

which is an object of interest for empirical process theory in general. Its concentration can also be seen as a non-asymptotic version of the Wilks phenomenon, which is another reason for tackling the theoretical challenge of proving that  $p_2(m)$  concentrates around some deterministic quantity. Section 5.2.3 reviews such theoretical results.

Handling large collections of estimators—see Sections 4.7 and 8.3.4—induces additional issues, since we cannot expect  $p_1(m)$ ,  $p_2(m)$ , and  $\delta(m)$  to concentrate tightly *uniformly* over all  $m \in \mathcal{M}$ . This raises the challenge of understanding precisely their uniform deviations among such large collections, with high-probability upper *and lower* bounds on these deviations. In the case of model selection, by grouping models of the same dimension as explained in Section 4.7, this problem reduces to concentrating  $p_1(m)$  and  $p_2(m)$  for empirical risk minimizers over models that are *unions* of a large number of vector spaces of the same dimension. Note that the same probabilistic challenge arises in the problem of understanding the overpenalization phenomenon—see Section 8.4—, for both large and small collections of estimators.

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## Appendix A: Some proofs

### A.1. Proof of Proposition 1

**Proof of Eq. (61) and (62)** By definition of  $\widehat{m}_{\min}^{(0)}(C)$ , for every  $m \in \mathcal{M}$ ,

$$\mathcal{R}\left(s_{\widehat{m}_{\min}^{(0)}(C)}^*\right) - \delta\left(\widehat{m}_{\min}^{(0)}(C)\right) + (C-1)p_2\left(\widehat{m}_{\min}^{(0)}(C)\right) \leq \mathcal{R}(s_m^*) - \delta(m) + (C-1)p_2(m)$$

hence

$$\begin{aligned} (1-C)p_2\left(\widehat{m}_{\min}^{(0)}(C)\right) &\geq \mathcal{R}\left(s_{\widehat{m}_{\min}^{(0)}(C)}^*\right) - \mathcal{R}(s^*) - [\mathcal{R}(s_m^*) - \mathcal{R}(s^*)] \\ &\quad + \delta(m) - \delta\left(\widehat{m}_{\min}^{(0)}(C)\right) + (1-C)p_2(m) \end{aligned}$$

which implies, using Eq. (60), that

$$(1-C)p_2\left(\widehat{m}_{\min}^{(0)}(C)\right) \geq -2[\mathcal{R}(s_m^*) - \mathcal{R}(s^*)] + (1-C)p_2(m) - \varepsilon'_\delta$$

hence Eq. (61) by dividing by  $(1-C)$ . Eq. (62) is a straightforward consequence of Eq. (61) since  $p_2(m_1) > 0$ .

**General proof of Eq. (60)** Let us assume that  $\xi_1, \dots, \xi_n \in \mathcal{X}$  are i.i.d. and some contrast function  $\gamma: \mathbb{E} \times \mathbb{S} \rightarrow \mathbb{R}$  and constants  $A, L > 0$  exist such that Eq. (63)–(65) hold true. Then, for every  $x \geq 0$ , with probability at least  $1 - 2 \text{card}(\mathcal{M})e^{-x}$ , for every  $\theta > 0$ , Eq. (60) holds with

$$\varepsilon_\delta = \theta \quad \text{and} \quad \varepsilon'_\delta = 2 \left( \frac{L}{2\theta} + \frac{2A}{3} \right) \frac{x}{n}.$$

Indeed, for every fixed  $m \in \mathcal{M}$ ,

$$\delta(m) - [\mathcal{R}(s^*) - \widehat{\mathcal{R}}_n(s^*)] = \frac{1}{n} \sum_{i=1}^n (X_{i,m} - \mathbb{E}[X_{i,m}]) \quad \text{where} \quad X_{i,m} = \gamma(\xi_i, s^*) - \gamma(\xi_i, s_m^*)$$

are i.i.d. random variables satisfying  $|X_{i,m}| \leq 2A$  almost surely. Therefore, by Bernstein's inequality (Boucheron et al., 2013, Theorem 2.10), for every  $x \geq 0$ , with probability at least  $1 - 2e^{-x}$ ,

$$\left| \delta(m) - [\mathcal{R}(s^*) - \widehat{\mathcal{R}}_n(s^*)] \right| \leq \sqrt{\frac{2x \text{var}(X_{i,m})}{n}} + \frac{2Ax}{3n} \leq \theta(\mathcal{R}(s_m^*) - \mathcal{R}(s^*)) + \left( \frac{L}{2\theta} + \frac{2A}{3} \right) \frac{x}{n}$$

and the result follows by the union bound.  $\square$

**Extension** Note that assuming only that  $(1 - \varepsilon_0)p_2(m) \leq \text{pen}_0(m) \leq (1 + \varepsilon_0)p_2(m)$  for some  $\varepsilon_0 \in [0, 1)$  with  $C(1 - \varepsilon_0) < 1$ —which implies  $p_2(m) \geq 0$ —, instead of Eq. (61) we get that

$$p_2(\widehat{m}_{\min}^{(0)}(C)) \geq \sup_{m \in \mathcal{M}} \left\{ \frac{1 - (1 + \varepsilon_0)C}{1 - (1 - \varepsilon_0)C} p_2(m) - \frac{2[\mathcal{R}(s_m^*) - \mathcal{R}(s^*)]}{1 - (1 - \varepsilon_0)C} \right\} - \frac{\varepsilon'_\delta}{1 - (1 - \varepsilon_0)C}.$$

If in addition some  $m_1 \in \mathcal{M}$  exists such that  $\mathcal{R}(s_{m_1}^*) = \mathcal{R}(s^*)$  and  $p_2(m_1) > 0$ , we get that for any  $\alpha \in (0, 1)$ ,

$$p_2(\widehat{m}_{\min}^{(0)}(C)) \geq (1 - \alpha)p_2(m_1)$$

if

$$C \leq 1 - \eta_\alpha \quad \text{where} \quad \eta_\alpha := 1 - \left( 1 - \frac{\varepsilon'_\delta}{\alpha p_2(m_1)} \right) \left[ 1 + \varepsilon_0 \left( \frac{2}{\alpha} - 1 \right) \right]^{-1}.$$

## A.2. Proof of Proposition 2

By definition of  $\widehat{m}_{\min}^{(0)}(C)$ , for every  $m \in \mathcal{M}$  and  $C > 1$ ,

$$\begin{aligned} & \mathcal{R}(\widehat{s}_{\widehat{m}_{\min}^{(0)}(C)}) - p_1(\widehat{m}_{\min}^{(0)}(C)) - \delta(\widehat{m}_{\min}^{(0)}(C)) + (C - 1)p_2(\widehat{m}_{\min}^{(0)}(C)) \\ & \leq \mathcal{R}(\widehat{s}_m) - p_1(m) - \delta(m) + (C - 1)p_2(m) \end{aligned}$$

hence, using Eq. (66),

$$\begin{aligned} & \mathcal{R}(\widehat{s}_{\widehat{m}_{\min}^{(0)}(C)}) - \mathcal{R}(s^*) + [(C - 1)(1 - \varepsilon_p) - 1]p_1(\widehat{m}_{\min}^{(0)}(C)) \\ & \leq \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*) + [(C - 1)(1 + \varepsilon_p) - 1]p_1(m) + \delta(\widehat{m}_{\min}^{(0)}(C)) - \delta(m). \end{aligned}$$

By Eq. (60), we get that for every  $m \in \mathcal{M}$  and  $C > 1$ ,

$$\begin{aligned} & \mathcal{R}(\widehat{s}_{\widehat{m}_{\min}^{(0)}(C)}) - \mathcal{R}(s^*) + [(C - 1)(1 - \varepsilon_p) - 1]p_1(\widehat{m}_{\min}^{(0)}(C)) - \varepsilon_\delta \left[ \mathcal{R}(s_{\widehat{m}_{\min}^{(0)}(C)}^*) - \mathcal{R}(s^*) \right] \\ & \leq \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*) + [(C - 1)(1 + \varepsilon_p) - 1]p_1(m) + \varepsilon_\delta [\mathcal{R}(s_m^*) - \mathcal{R}(s^*)] + \varepsilon'_\delta \end{aligned}$$



that is,

$$\begin{aligned} & \left(1 - \max\{1 - (C-1)(1 - \varepsilon_p), \varepsilon_\delta\}\right) \left[ \mathcal{R}\left(\widehat{s}_{\widehat{m}_{\min}^{(0)}(C)}\right) - \mathcal{R}(s^*) \right] \\ & \leq \left(1 + \max\{(C-1)(1 + \varepsilon_p) - 1, \varepsilon_\delta\}\right) \inf_{m \in \mathcal{M}} \left\{ \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*) \right\} + \varepsilon'_\delta \end{aligned}$$

which proves Eq. (67). Using again Eq. (66), we get

$$\begin{aligned} p_2\left(\widehat{m}_{\min}^{(0)}(C)\right) & \leq (1 + \varepsilon_p) p_1\left(\widehat{m}_{\min}^{(0)}(C)\right) \leq (1 + \varepsilon_p) \left[ \mathcal{R}\left(\widehat{s}_{\widehat{m}_{\min}^{(0)}(C)}\right) - \mathcal{R}(s^*) \right] \\ & \leq K(C)(1 + \varepsilon_p) \inf_{m \in \mathcal{M}} \left\{ \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*) \right\} + K'(C)(1 + \varepsilon_p). \quad \square \end{aligned}$$

**Extension** Note that if  $\text{pen}_0(m) = p_2(m)$  is replaced by

$$(1 - \varepsilon_0)p_2(m) \leq \text{pen}_0(m) \leq (1 + \varepsilon_0)p_2(m)$$

for some  $\varepsilon_0 \geq 0$  with  $C(1 - \varepsilon_0) > 1$ , and if Eq. (66) is replaced by

$$\forall m \in \mathcal{M}, \quad -\varepsilon'_p + \varepsilon_p^- p_1(m) \leq p_2(m) \leq \varepsilon_p^+ p_1(m) + \varepsilon'_p \quad (84)$$

for some  $\varepsilon_p^-, \varepsilon_p^+ > 0$  and  $\varepsilon'_p \geq 0$ , the same proof shows that Eq. (67) holds true with

$$\begin{aligned} K(C) & := \frac{\max\{[C(1 + \varepsilon_0) - 1]\varepsilon_p^+, 1 + \varepsilon_\delta\}}{\min\{[C(1 - \varepsilon_0) - 1]\varepsilon_p^-, 1 - \varepsilon_\delta\}} \\ \text{and} \quad K'(C) & := \frac{\varepsilon'_\delta + 2(C-1)\varepsilon_p'}{\min\{[C(1 - \varepsilon_0) - 1]\varepsilon_p^-, 1 - \varepsilon_\delta\}}, \end{aligned}$$

and Eq. (68) replaced by

$$p_2\left(\widehat{m}_{\min}^{(0)}(C)\right) \leq K(C)\varepsilon_p^+ \inf_{m \in \mathcal{M}} \left\{ \mathcal{R}(\widehat{s}_m) - \mathcal{R}(s^*) \right\} + K'(C)\varepsilon_p^+ + \varepsilon'_p. \quad (85)$$

### A.3. Proof of Proposition 3

We first state two general lemmas for  $\widehat{C}_{\text{thr}}$  and  $\widehat{C}_{\text{window}}$ , as defined by Eq. (20) and (19) in Section 2.5, respectively. These lemmas do not assume a specific definition for  $\widehat{m}(C)$  and  $D_m$ , so they apply to Algorithms 1, 3, 4, and 5 (possibly up to a rescaling of  $\mathcal{C}_m$  for Lemma 2 and Algorithm 5).

**Lemma 1.** *Let  $T_n \in \mathbb{R}$ ,  $\widehat{m}: [0, +\infty) \rightarrow \mathcal{M}$  some function, and  $\widehat{C}_{\text{thr}}(T_n) := \inf\{C \geq 0 / D_{\widehat{m}(C)} \leq T_n\}$ . If  $\Gamma_1 \geq 0$  and  $D_{\widehat{m}(C)} > T_n$  for all  $C < \Gamma_1$ , then,  $\widehat{C}_{\text{thr}}(T_n) \geq \Gamma_1$ . If  $\Gamma_2 \geq 0$  and  $D_{\widehat{m}(\Gamma_2)} \leq T_n$ , then,  $\widehat{C}_{\text{thr}}(T_n) \leq \Gamma_2$ .*

*Proof.* The proof is straightforward from the definition of  $\widehat{C}_{\text{thr}}$ . □



**Lemma 2.** Let  $\eta > 0$ ,  $\widehat{m} : [0, +\infty) \rightarrow \mathcal{M}$  some function, and

$$\widehat{C}_{\text{window}}(\eta) \in \operatorname{argmax}_{C \geq 0} \{D_{\widehat{m}(C/[1+\eta])} - D_{\widehat{m}(C[1+\eta])}\}.$$

Assume that  $0 \leq D_m \leq n$  for every  $m \in \mathcal{M}$ . Assume in addition that  $a_n, b_n \in \mathbb{R}$  and  $\Gamma_2 > \Gamma_1 > 0$  exist such that  $a_n - b_n > \max\{n - a_n, b_n\}$ ,

$$\forall C \leq \Gamma_1, \quad D_{\widehat{m}(C)} \geq a_n, \quad \forall C \geq \Gamma_2, \quad D_{\widehat{m}(C)} \leq b_n, \quad \text{and} \quad (1 + \eta)^2 \geq \frac{\Gamma_2}{\Gamma_1}.$$

Then, we have

$$\frac{\Gamma_1}{1 + \eta} < \widehat{C}_{\text{window}}(\eta) < \Gamma_2(1 + \eta).$$

*Proof.* First, for  $C = \sqrt{\Gamma_1 \Gamma_2}$ , we have  $C/(1 + \eta) \leq \Gamma_1$  and  $C(1 + \eta) \geq \Gamma_2$ , hence we obtain  $D_{\widehat{m}(C/[1+\eta])} - D_{\widehat{m}(C[1+\eta])} \geq a_n - b_n$ . Second, for every  $C \leq \Gamma_1/(1 + \eta)$ , we have the inequality  $D_{\widehat{m}(C/[1+\eta])} - D_{\widehat{m}(C[1+\eta])} \leq n - a_n$ . Third, for any  $C \geq \Gamma_2(1 + \eta)$ ,  $D_{\widehat{m}(C/[1+\eta])} - D_{\widehat{m}(C[1+\eta])} \leq b_n$ . The result follows since  $a_n - b_n > \max\{n - a_n, b_n\}$ .  $\square$

Let us now prove Proposition 3.

By Eq. (30) and Eq. (35) in the proof of Theorem 1, for all  $x \geq 0$ , on the event  $\Omega_x$  which has a probability larger than  $1 - 4\operatorname{card}(\mathcal{M})e^{-x}$ , we have

$$\forall C \leq C_1(x; a_n), \quad D_{\widehat{m}(C)} \geq a_n \quad \text{and} \quad \forall C \geq C_2(x; b_n; c_n), \quad D_{\widehat{m}(C)} \leq b_n, \quad (86)$$

whatever  $0 \leq c_n < b_n \leq n$  and  $0 \leq a_n < n$ , provided that  $\mathcal{M}$  contains at least one model of dimension at most  $c_n$ .

**Proof of Eq. (75)** First, note that

$$C_1\left(x; \frac{2n}{3}\right) = \sigma^2 \left[ 1 - \left( 12\sqrt{\frac{x}{n}} + 18\frac{x}{n} \right) \right] > 0$$

since  $\sqrt{x/n} \leq (\sqrt{6} - 2)/6$ . Therefore, by continuity of  $C_1$  and using that  $c_n < n/3$ , there exists some  $\varepsilon_1 \in (0, \min\{1/2, 1 - 3c_n/n\})$  such that  $C_1(x; \frac{2n}{3}(1 + \varepsilon)) > 0$  for any  $\varepsilon \in [0, \varepsilon_1]$ . Let us take any  $\varepsilon \in (0, \varepsilon_1]$ ,  $a_n = \frac{2n}{3}(1 + \varepsilon) \in (2n/3, n)$ , and  $b_n = \frac{n}{3}(1 - \varepsilon) \in (c_n, n/3)$ . By Lemma 2 with  $a_n, b_n$  as above,  $\Gamma_1 = C_1(x; a_n)$ , and  $\Gamma_2 = C_2(x; b_n; c_n)$ , on  $\Omega_x$ , since Eq. (86) holds true, we get that

$$\forall \eta \geq \sqrt{\frac{C_2(x; \frac{n}{3}(1 - \varepsilon); c_n)}{C_1(x; \frac{2n}{3}(1 + \varepsilon))}} - 1, \quad \frac{C_1(x; \frac{2n}{3}(1 + \varepsilon))}{1 + \eta} < \widehat{C}_{\text{window}}(\eta) < C_2\left(x; \frac{n}{3}(1 - \varepsilon); c_n\right)(1 + \eta).$$

Now, since  $z \mapsto C_1(x; z)$  is continuous and different from zero at  $z = 2n/3$ , and since the mapping  $z \mapsto C_2(x; z; c_n)$  is continuous at  $z = n/3$  (using that  $c_n < n/3$ ), for any

$$\eta > \sqrt{\frac{C_2(x; \frac{n}{3}; c_n)}{C_1(x; \frac{2n}{3})}} - 1,$$

some  $\varepsilon_2 \in (0, \varepsilon_1]$  exists such that

$$\forall \varepsilon \in (0, \varepsilon_2], \quad \eta \geq \sqrt{\frac{C_2(x; \frac{n}{3}(1-\varepsilon); c_n)}{C_1(x; \frac{2n}{3}(1+\varepsilon))}} - 1.$$

So, for such  $\eta$ , on  $\Omega_x$ , for every  $\varepsilon \in (0, \varepsilon_2]$ ,

$$\frac{C_1(x; \frac{2n}{3}(1+\varepsilon))}{1+\eta} < \widehat{C}_{\text{window}}(\eta) < C_2(x; \frac{n}{3}(1-\varepsilon); c_n)(1+\eta).$$

Making  $\varepsilon$  tend to zero in the above inequality yields the result.

**Proof of Eq. (76)** For any  $a_n \in (T_n, n)$ , by Eq. (86), on  $\Omega_x$ , we have  $D_{\widehat{m}(C)} \geq a_n > T_n$  for every  $C \leq C_1(x; a_n)$ , hence  $\widehat{C}_{\text{thr.}}(T_n) \geq C_1(x; a_n)$  by Lemma 1 with  $\Gamma_1 = C_1(x; a_n)$ . So, on  $\Omega_x$ ,

$$\widehat{C}_{\text{thr.}}(T_n) \geq \sup_{a_n \in (T_n, n)} \{C_1(x; a_n)\} = C_1(x; T_n).$$

By Eq. (86) with  $b_n = T_n > c_n$ , on  $\Omega_x$  we have  $D_{\widehat{m}(C)} \leq T_n$  for every  $C \geq C_2(x; T_n; c_n)$ , hence  $\widehat{C}_{\text{thr.}}(T_n) \leq C_2(x; T_n; c_n)$  by Lemma 1 with  $\Gamma_2 = C_2(x; T_n; c_n)$ .

**Proof of Eq. (77)** Let  $\alpha = \log(4 \text{card } \mathcal{M}) \geq \log(8)$ , since  $\text{card}(\mathcal{M}) \geq 2$  under the assumptions of Proposition 3. For every  $z \geq 0$ , by Eq. (76) with  $x = z + \alpha$  and  $c_n$  replaced by  $T_n/2$ ,

$$\begin{aligned} \mathbb{P} \left( \left( \widehat{C}_{\text{thr.}} - \sigma^2 \right)^2 \geq 4 \max \left\{ \left( 1 - \frac{T_n}{n} \right)^{-2}, \left( \frac{T_n}{2n} \right)^{-2} \right\} \right. \\ \left. \times \left[ \mathcal{B} \left( \frac{T_n}{2} \right) + 2\sigma^2 \left( \sqrt{\frac{z+\alpha}{n}} + \frac{2(z+\alpha)}{n} \right) \right]^2 \right) \leq e^{-z}. \end{aligned} \quad (87)$$

Then, integrating Eq. (87) with respect to  $z$ —that is, using Lemma 3 below—we get that Eq. (77) holds true. Note that much smaller constants can be obtained by assuming that  $\text{card}(\mathcal{M})$  is large enough, or that  $\log(\text{card } \mathcal{M})/n$  is small enough. For instance, under the assumption that  $100 \leq \text{card}(\mathcal{M}) \leq \exp(n/100)$ , we get

$$\mathbb{E} \left[ \left( \widehat{C}_{\text{thr.}} - \sigma^2 \right)^2 \right] \leq \max \left\{ \left( 1 - \frac{T_n}{n} \right)^{-2}, \left( \frac{T_n}{2n} \right)^{-2} \right\} \left[ 12\mathcal{B} \left( \frac{T_n}{2} \right)^2 + \frac{102\sigma^4 \log(\text{card } \mathcal{M})}{n} \right].$$

□

**Lemma 3.** For a real-valued random variable  $Z$ , if some  $a, b, c \geq 0$  exist such that for every  $z \geq 0$ ,

$$\begin{aligned} \mathbb{P}(Z \geq a + bz + cz^2) &\leq e^{-z}, \\ \text{then, } \mathbb{E}[Z] &\leq a + 2b + 4c. \end{aligned}$$

Lemma 3 is a classical integration exercise.

#### A.4. Computations about $\widehat{\sigma}_{m_0}^2$

The following proposition gives a general formula for the variance and MSE of the residual-variance estimator  $\widehat{\sigma}_{m_0}^2$  defined by Eq. (71) in Section 6.1. Note that Proposition 4 and Lemma 4 below are classical results (see for instance Ullah and Zinde-Walsh, 1992, Eq. (5), or Dette et al., 1998, Eq. (6)). We state and prove them here for completeness.

In this subsection, for any matrix  $M \in \mathcal{M}_n(\mathbb{R})$ ,  $\text{diag}(M)$  denotes the diagonal matrix of the diagonal elements of  $M$  and  $\mathbf{1} = (1, \dots, 1) \in \mathbb{R}^n$ .

**Proposition 4.** *Let  $\Pi \in \mathcal{M}_n(\mathbb{R})$  some orthogonal projection matrix such that  $D = \text{tr}(\Pi) < n$ ,  $\varepsilon \in \mathbb{R}^n$  some random vector with independent components, and  $F \in \mathbb{R}^n$ . Assume that for all  $i \in \{1, \dots, n\}$ ,*

$$\mathbb{E}[\varepsilon_i] = 0, \quad \mathbb{E}[\varepsilon_i^2] = \sigma^2, \quad \mathbb{E}[\varepsilon_i^3] = m_3, \quad \text{and} \quad \mathbb{E}[\varepsilon_i^4] = m_4.$$

Let

$$\widehat{\sigma}^2 := \frac{1}{n-D} \|(I_n - \Pi)(F + \varepsilon)\|^2.$$

Then,

$$\text{var}(\widehat{\sigma}^2) = V + \frac{4\|(I_n - \Pi)F\|^2 \sigma^2}{(n-D)^2} + \frac{4\langle F, (I_n - \Pi) \text{diag}(I_n - \Pi) \mathbf{1} \rangle}{(n-D)^2} m_3 \quad (88)$$

$$\text{where } V := \frac{1}{(n-D)^2} \left( \sum_{i=1}^n (1 - \Pi_{i,i})^2 \right) (m_4 - 3\sigma^4) + \frac{2}{n-D} \sigma^4,$$

$$\text{and } \mathbb{E}[(\widehat{\sigma}^2 - \sigma^2)^2] = V + \frac{4\|(I_n - \Pi)F\|^2 \sigma^2}{(n-D)^2} + \frac{\|(I_n - \Pi)F\|^4}{(n-D)^2} + \frac{4\langle F, (I_n - \Pi) \text{diag}(I_n - \Pi) \mathbf{1} \rangle}{(n-D)^2} m_3. \quad (89)$$

In particular, if the  $\varepsilon_i$  are Gaussian,

$$\text{var}(\widehat{\sigma}^2) = \frac{2\sigma^4}{n-D} + \frac{4\|(I_n - \Pi)F\|^2}{(n-D)^2} \sigma^2 \quad (90)$$

$$\mathbb{E}[(\widehat{\sigma}^2 - \sigma^2)^2] = \frac{2\sigma^4}{n-D} + \frac{4\|(I_n - \Pi)F\|^2}{(n-D)^2} \sigma^2 + \frac{\|(I_n - \Pi)F\|^4}{(n-D)^2}. \quad (91)$$

*Proof of Proposition 4.* Applying Lemma 4 below with  $M = I_n - \Pi$  yields Eq. (88), since we have  $\widehat{\sigma}^2 = Z/(n-D)$  and  $M$  is an orthogonal projection matrix with  $\text{tr}(M) = n-D$ . Eq. (89) follows, in combination with Eq. (72), since

$$\mathbb{E}[(\widehat{\sigma}^2 - \sigma^2)^2] = \left( \mathbb{E}[\widehat{\sigma}^2] - \sigma^2 \right)^2 + \text{var}(\widehat{\sigma}^2).$$

In the Gaussian case,  $m_3 = 0$  and  $m_4 = 3\sigma^4$ , hence

$$V = \frac{2\sigma^4}{n-D},$$

which leads to Eq. (90) and (91). □

**Lemma 4.** Let  $F \in \mathbb{R}^n$ ,  $M \in \mathcal{M}_n(\mathbb{R})$  a symmetric matrix,  $\varepsilon \in \mathbb{R}^n$  some random vector with independent components such that for all  $i \in \{1, \dots, n\}$ ,

$$\mathbb{E}[\varepsilon_i] = 0, \quad \mathbb{E}[\varepsilon_i^2] = \sigma^2, \quad \mathbb{E}[\varepsilon_i^3] = m_3, \quad \text{and} \quad \mathbb{E}[\varepsilon_i^4] = m_4.$$

Then, if  $Z = \langle F + \varepsilon, M(F + \varepsilon) \rangle$ ,

$$\text{var}(Z) = W + 4\|MF\|^2\sigma^2 + 4\langle F, M \text{diag}(M)\mathbf{1} \rangle m_3 \quad (92)$$

$$\text{where} \quad W := \text{tr}(\text{diag}(M)^2) (m_4 - 3\sigma^4) + 2\text{tr}(M^2)\sigma^4$$

$$\text{satisfies} \quad 0 \leq W \leq (2\sigma^4 + m_4) \text{tr}(M^2). \quad (93)$$

*Proof of Lemma 4.* First note that

$$Z = \langle F, MF \rangle + \langle \varepsilon, M\varepsilon \rangle + 2\langle MF, \varepsilon \rangle.$$

Then,

$$\mathbb{E}[Z] = \langle F, MF \rangle + \mathbb{E}[\langle \varepsilon, M\varepsilon \rangle] = \langle F, MF \rangle + \sigma^2 \text{tr}(M).$$

Furthermore,

$$\begin{aligned} \mathbb{E}[Z^2] &= \langle F, MF \rangle^2 + \mathbb{E}[\langle \varepsilon, M\varepsilon \rangle^2] + 4\mathbb{E}[\langle MF, \varepsilon \rangle^2] \\ &\quad + 2\langle F, MF \rangle \sigma^2 \text{tr}(M) + 4\mathbb{E}[\langle \varepsilon, M\varepsilon \rangle \langle MF, \varepsilon \rangle] \\ &= \langle F, MF \rangle^2 + \left( \sum_{i=1}^n M_{i,i}^2 \right) (m_4 - 3\sigma^4) + \left[ \text{tr}(M)^2 + 2\text{tr}(M^\top M) \right] \sigma^4 \\ &\quad + 4\|MF\|^2\sigma^2 + 2\langle F, MF \rangle \sigma^2 \text{tr}(M) + 4 \left( \sum_{i,j=1}^n M_{i,i} M_{i,j} F_j \right) m_3 \end{aligned}$$

where we used that

$$\begin{aligned} \mathbb{E}[\langle \varepsilon, M\varepsilon \rangle^2] &= \mathbb{E} \left[ \left( \sum_{i,j} \varepsilon_i M_{i,j} \varepsilon_j \right)^2 \right] = \sum_{i,j,k,\ell} M_{i,j} M_{k,\ell} \mathbb{E}[\varepsilon_i \varepsilon_j \varepsilon_k \varepsilon_\ell] \\ &= \left( \sum_{i=1}^n M_{i,i}^2 \right) (m_4 - 3\sigma^4) + \left( \text{tr}(M)^2 + \text{tr}(M^2) + \text{tr}(M^\top M) \right) \sigma^4 \end{aligned}$$

and for any  $G \in \mathbb{R}^n$  (here,  $G = MF$ ),

$$\mathbb{E}[\langle G, \varepsilon \rangle^2] = \|G\|^2 \sigma^2$$

$$\text{and} \quad \mathbb{E}[\langle \varepsilon, M\varepsilon \rangle \langle G, \varepsilon \rangle] = \mathbb{E} \left[ \sum_{i,j,k} \varepsilon_i M_{i,j} \varepsilon_j G_k \varepsilon_k \right] = \left( \sum_{i=1}^n M_{i,i} G_i \right) m_3.$$

Eq. (92) follows since  $M$  is symmetric,  $\text{var}(Z) = \mathbb{E}[Z^2] - \mathbb{E}[Z]^2$ ,

$$\sum_{i,j=1}^n M_{i,i} M_{i,j} F_j = \langle F, M^\top \text{diag}(M)\mathbf{1} \rangle \quad \text{and} \quad \sum_{i=1}^n M_{i,i}^2 = \text{tr}(\text{diag}(M)^2).$$

For proving Eq. (93), we remark that

$$W = \text{tr}(\widehat{\text{diag}}(M)^2)(m_4 - \sigma^4) + 2 \left[ \text{tr}(M^2) - \text{tr}(\widehat{\text{diag}}(M)^2) \right] \sigma^4, \\ m_4 \geq \sigma^4, \quad \text{and} \quad 0 \leq \text{tr}(\widehat{\text{diag}}(M)^2) \leq \text{tr}(M^2)$$

since  $M$  is symmetric.  $\square$

## Appendix B: Algorithms

### B.1. Computation of the full path $(\widehat{m}(C))_{C \geq 0}$ in Algorithms 1, 3, 4, and 5

One can formulate the first step in Algorithms 1, 3, 4, and 5 as computing, for every  $C \geq 0$ ,

$$\widehat{m}(C) \in \underset{m \in \mathcal{M}}{\text{argmin}} \{f(m) + Cg(m)\} \quad (94)$$

for some functions  $f, g : \mathcal{M} \rightarrow \mathbb{R}$ , where  $\mathcal{M}$  is assumed to be finite. In the most general case (Algorithm 5),  $f(m) = \widehat{\mathcal{R}}_n(\widehat{s}_m)$  and  $g(m) = \text{pen}_0(m)$ . Particular cases (Algorithms 1, 3, and 4) follow.

This subsection explains how to compute the full path  $(\widehat{m}(C))_{C \geq 0}$  defined by Eq. (94), given  $(f(m))_{m \in \mathcal{M}}$  and  $(g(m))_{m \in \mathcal{M}}$ , with at most  $\mathcal{O}([\text{card } \mathcal{M}]^2)$  operations, and much less in practice. The material presented here is adapted from Arlot and Massart (2009, Section 3.2). Similar results —with a bit less details and formulated in specific frameworks where  $\mathcal{M} \subset \mathbb{N}$ — have been proved earlier by Lebarbier (2002, Lemma 4.4.1), Lavielle (2005, Proposition 2.1) and Zwald (2005, Section 6.4.3).

First, remark that the definition (94) of  $\widehat{m}(C)$  can be ambiguous. Let us choose a strict total order  $\prec$  on  $\mathcal{M}$  such that  $g$  is non-decreasing, which is always possible since  $\mathcal{M}$  is finite. Then, by convention, for every  $C \geq 0$ ,  $\widehat{m}(C)$  is defined as

$$\widehat{m}(C) = \min_{\prec} \mathcal{E}(C) \quad \text{where} \quad \mathcal{E}(C) := \underset{m \in \mathcal{M}}{\text{argmin}} \{f(m) + Cg(m)\}. \quad (95)$$

The main reason why the whole trajectory  $(\widehat{m}(C))_{C \geq 0}$  can be computed efficiently is its particular shape. Indeed, the proof of Proposition 5 below shows that  $C \mapsto \widehat{m}(C)$  is piecewise constant and non-increasing for  $\prec$ . Then, the whole trajectory  $(\widehat{m}(C))_{C \geq 0}$  can be written as

$$\forall i \in \{0, \dots, i_{\max}\}, \quad \forall C \in [C_i, C_{i+1}), \quad \widehat{m}(C) = m_i \quad (96)$$

where  $i_{\max} \in \{0, \dots, \text{card}(\mathcal{M}) - 1\}$  is the number of jumps,  $(C_i)_{0 \leq i \leq i_{\max} + 1}$  is an increasing sequence of non-negative reals (the location of the jumps) with  $C_0 = 0$  and  $C_{i_{\max} + 1} = +\infty$ , and  $(m_i)_{0 \leq i \leq i_{\max}}$  is a non-increasing sequence of elements of  $\mathcal{M}$ .

**Algorithm 7.** Input:  $(f(m))_{m \in \mathcal{M}}$ ,  $(g(m))_{m \in \mathcal{M}}$ , and  $\prec$  some strict total order on  $\mathcal{M}$  such that  $g$  is non-decreasing.

Initialization:  $C_0 := 0$  and  $m_0 := \min_{\prec} \underset{m \in \mathcal{M}}{\text{argmin}} \{f(m)\}$ .

Step  $i$ ,  $i \geq 1$ : Let

$$\mathcal{G}(m_{i-1}) := \{m \in \mathcal{M} \text{ s.t. } f(m) > f(m_{i-1}) \quad \text{and} \quad g(m) < g(m_{i-1})\}.$$

If  $\mathcal{G}(m_{i-1}) = \emptyset$ , then put  $C_i = +\infty$ ,  $i_{\max} = i - 1$  and stop. Otherwise, define

$$C_i := \min \left\{ \frac{f(m) - f(m_{i-1})}{g(m_{i-1}) - g(m)} \text{ s.t. } m \in \mathcal{G}(m_{i-1}) \right\} \quad (97)$$

$$\text{and } m_i := \min_{\prec} \mathcal{F}_i \quad \text{with } \mathcal{F}_i := \operatorname{argmin}_{m \in \mathcal{G}(m_{i-1})} \left\{ \frac{f(m) - f(m_{i-1})}{g(m_{i-1}) - g(m)} \right\}.$$

**Output:**  $(C_i)_{0 \leq i \leq i_{\max}+1}$  and  $(m_i)_{0 \leq i \leq i_{\max}}$ , which describe according to Eq. (96) the full trajectory  $(\widehat{m}(C))_{C \geq 0}$  defined by Eq. (95).

**Proposition 5** (Correctness of Algorithm 7). *For every  $C \geq 0$ , let  $\widehat{m}(C)$  be defined by Eq. (95). Assume  $\mathcal{M}$  is finite. Then, Algorithm 7 terminates and  $i_{\max} \leq \operatorname{card}(\mathcal{M}) - 1$ . Furthermore, Algorithm 7 is correct, that is,  $(C_i)_{0 \leq i \leq i_{\max}+1}$  is increasing and  $\forall i \in \{0, \dots, i_{\max} - 1\}$ ,  $\forall C \in [C_i, C_{i+1})$ ,  $\widehat{m}(C) = m_i$ .*

Proposition 5 also gives an upper bound on the computational complexity of Algorithm 7: since the complexity of each step is  $\mathcal{O}(\operatorname{card}(\mathcal{M}))$ , the complexity of Algorithm 7 is upper-bounded by  $\mathcal{O}(i_{\max} \operatorname{card}(\mathcal{M})) \leq \mathcal{O}([\operatorname{card}(\mathcal{M})]^2)$ . In general, this upper bound is pessimistic since we usually have  $i_{\max} \ll \operatorname{card}(\mathcal{M})$  in practice.

*Proof of Proposition 5.* First, since  $\mathcal{M}$  is finite,  $\mathcal{G}(m_{i-1})$  is also finite and  $m_i$  is well-defined as soon as  $\mathcal{G}(m_{i-1}) \neq \emptyset$ , which holds for every  $i \leq i_{\max}$ . Moreover, by construction,  $g(m_i)$  decreases with  $i$ , so that all the  $m_i \in \mathcal{M}$  are different; hence, Algorithm 7 terminates and we have the inequality  $i_{\max} + 1 \leq \operatorname{card}(\mathcal{M})$ . Notice also that  $C_i$  can always be defined by Eq. (97) with the convention  $\min \emptyset = +\infty$ .

We now prove by induction that the following property holds true for every  $i \in \{0, \dots, i_{\max}\}$ , which implies that Proposition 5 holds true:

$$\mathcal{P}_i : \quad C_i < C_{i+1} \quad \text{and} \quad \forall C \in [C_i, C_{i+1}), \quad \widehat{m}(C) = m_i.$$

**$\mathcal{P}_0$  holds true** By definition of  $C_1$ , since  $\mathcal{M}$  is finite,  $C_1 > 0$ . Note that  $C_1$  may be equal to  $+\infty$  if  $\mathcal{G}(m_0) = \emptyset$ . For  $C = C_0 = 0$ , the definition of  $m_0$  is the one of  $\widehat{m}(0)$ , so that  $\widehat{m}(C) = m_0$ . For  $C \in (0, C_1)$ , Lemma 5 below shows that either  $\widehat{m}(C) = \widehat{m}(0) = m_0$  or  $\widehat{m}(C) \in \mathcal{G}(m_0)$ . In the latter case, by definition of  $C_1$ ,

$$\frac{f(\widehat{m}(C)) - f(m_0)}{g(m_0) - g(\widehat{m}(C))} \geq C_1 > C$$

hence

$$f(\widehat{m}(C)) + Cg(\widehat{m}(C)) > f(m_0) + Cg(m_0)$$

which contradicts the definition of  $\widehat{m}(C)$ . Therefore,  $\mathcal{P}_0$  holds true.

**$\mathcal{P}_i \Rightarrow \mathcal{P}_{i+1}$  for every  $i \in \{0, \dots, i_{\max} - 1\}$**  Assume that  $\mathcal{P}_i$  holds true. First, we have to prove that  $C_{i+2} > C_{i+1}$ . If  $i = i_{\max} - 1$ , this is clear since  $C_{i_{\max}+1} = +\infty$ . Otherwise,  $C_{i+2} < +\infty$  and  $m_{i+2}$  exists. Then, by definition of  $m_{i+2}$  and  $C_{i+2}$  (resp.  $m_{i+1}$  and  $C_{i+1}$ ), we have

$$f(m_{i+2}) - f(m_{i+1}) = C_{i+2} [g(m_{i+1}) - g(m_{i+2})] \quad (98)$$

$$f(m_{i+1}) - f(m_i) = C_{i+1} [g(m_i) - g(m_{i+1})]. \quad (99)$$

Moreover,  $m_{i+2} \in \mathcal{G}(m_{i+1}) \subset \mathcal{G}(m_i)$  and  $m_{i+2} \prec m_{i+1}$  (because  $g$  is non-decreasing). Using again the definition of  $C_{i+1}$ , we have

$$f(m_{i+2}) - f(m_i) > C_{i+1} [g(m_i) - g(m_{i+2})] \quad (100)$$

(the inequality is strict: otherwise, we would have  $m_{i+2} \in \mathcal{F}_{i+1}$  and  $m_{i+2} \prec m_{i+1} = \min_{\prec} \mathcal{F}_{i+1}$ , which is not possible). The difference of Eq. (100) and (99) yields

$$f(m_{i+2}) - f(m_{i+1}) > C_{i+1} [g(m_{i+1}) - g(m_{i+2})].$$

By Eq. (98), we deduce that

$$C_{i+2} [g(m_{i+1}) - g(m_{i+2})] > C_{i+1} [g(m_{i+1}) - g(m_{i+2})],$$

hence  $C_{i+2} > C_{i+1}$  since  $g(m_{i+1}) > g(m_{i+2})$ .

Second, we prove that  $\widehat{m}(C_{i+1}) = m_{i+1}$ . From  $\mathcal{P}_i$ , we know that for every  $m \in \mathcal{M}$ , for every  $C \in [C_i, C_{i+1})$ ,  $f(m_i) + Cg(m_i) \leq f(m) + Cg(m)$ . Taking the limit when  $C$  tends to  $C_{i+1}$ , it follows that  $m_i \in \mathcal{E}(C_{i+1})$ . By Eq. (99), we then have  $m_{i+1} \in \mathcal{E}(C_{i+1})$ . Now, let  $m'$  be any element of  $\mathcal{E}(C_{i+1})$ . By Lemma 5 with  $C = C_i$ ,  $m = m_i = \widehat{m}(C_i) \in \mathcal{E}(C_i)$  and  $C' = C_{i+1} > C_i$ , we have either (a)  $f(m') = f(m_i)$  and  $g(m') = g(m_i)$  or (b)  $m' \in \mathcal{G}(m_i)$ ; case (c) is excluded since  $m_i = \widehat{m}(C_i)$ . In case (a),  $g(m') = g(m_i) > g(m_{i+1})$ , hence  $m_{i+1} \prec m'$  because  $g$  is non-decreasing. In case (b), notice that  $m_i, m' \in \mathcal{E}(C_{i+1})$  implies  $f(m') + C_{i+1}g(m') = f(m_i) + C_{i+1}g(m_i)$ . Since  $m' \in \mathcal{G}(m_i)$ , we get that  $m' \in \mathcal{F}_{i+1}$ . Then, by definition of  $m_{i+1}$ , we have  $m_{i+1} \preceq m'$ . Overall, we have proved that  $m_{i+1}$  belongs to  $\mathcal{E}(C_{i+1})$  and is smaller than any element  $m'$  of  $\mathcal{E}(C_{i+1})$ , which proves that  $m_{i+1} = \min_{\prec} \mathcal{E}(C_{i+1}) = \widehat{m}(C_{i+1})$ .

Let  $C' \in (C_{i+1}, C_{i+2})$ . It remains to prove  $\widehat{m}(C') = m_{i+1}$ . From the last statement of Lemma 5 with  $C = C_{i+1}$ , we have either  $\widehat{m}(C') = \widehat{m}(C_{i+1}) = m_{i+1}$  or  $\widehat{m}(C') \in \mathcal{G}(\widehat{m}(C_{i+1})) = \mathcal{G}(m_{i+1})$ . In the latter case (in which  $\mathcal{G}(m_{i+1}) \neq \emptyset$  hence  $C_{i+2} < \infty$ ), by definition of  $C_{i+2}$ ,

$$\frac{f(\widehat{m}(C')) - f(m_{i+1})}{g(m_{i+1}) - g(\widehat{m}(C'))} \geq C_{i+2} > C'$$

so that

$$f(\widehat{m}(C')) + C'g(\widehat{m}(C')) > f(m_{i+1}) + C'g(m_{i+1})$$

which contradicts the definition of  $\widehat{m}(C')$ . Therefore,  $\widehat{m}(C') = m_{i+1}$ , which ends proving  $\mathcal{P}_{i+1}$ .  $\square$

The following lemma is used in the proof of Proposition 5 above.

**Lemma 5.** *With the notation of Proposition 5 and its proof, if we have  $0 \leq C < C'$ ,  $m \in \mathcal{E}(C)$ , and  $m' \in \mathcal{E}(C')$ , then one of the following statements holds true:*

- (a)  $f(m) = f(m')$  and  $g(m) = g(m')$ .
- (b)  $f(m) < f(m')$  and  $g(m) > g(m')$ .
- (c)  $C = 0$ ,  $f(m) = f(m')$  and  $g(m) > g(m')$ , hence  $m \neq \widehat{m}(0)$ .

*In particular, for any  $0 \leq C < C'$ , we have either  $\widehat{m}(C) = \widehat{m}(C')$  or  $\widehat{m}(C') \in \mathcal{G}(\widehat{m}(C))$ .*



*Proof of Lemma 5.* By definition of  $\mathcal{E}(C)$  and  $\mathcal{E}(C')$ ,

$$f(m) + Cg(m) \leq f(m') + Cg(m') \quad (101)$$

$$\text{and} \quad f(m') + C'g(m') \leq f(m) + C'g(m). \quad (102)$$

Summing Eq. (101) and (102) gives  $(C' - C)g(m') \leq (C' - C)g(m)$  so that

$$g(m') \leq g(m). \quad (103)$$

Since  $C \geq 0$ , Eq. (101) and (103) give  $f(m) + Cg(m) \leq f(m') + Cg(m)$ , that is

$$f(m) \leq f(m'). \quad (104)$$

If  $g(m) = g(m')$ , Eq. (102) and (104) imply  $f(m') = f(m)$  hence (a) is satisfied. Otherwise,  $g(m) > g(m')$  by Eq. (103), and Eq. (101) implies  $f(m) < f(m')$  or  $C = 0$ . If  $f(m) < f(m')$ , (b) holds true. Otherwise,  $f(m) = f(m')$  and  $C = 0$ . Since  $g(m') < g(m)$ , we get  $m' \prec m$  hence  $m \neq \widehat{m}(0)$ .

The last statement follows by taking  $m = \widehat{m}(C)$  and  $m' = \widehat{m}(C')$ , which excludes case (c). In case (a),  $\mathcal{E}(C) = \mathcal{E}(C')$  hence  $\widehat{m}(C) = \widehat{m}(C')$ . In case (b),  $\widehat{m}(C') \in \mathcal{G}(\widehat{m}(C))$ .  $\square$

## B.2. Computation of $\widehat{C}_{\text{window}}$ in step 2 of Algorithms 1, 3, 4, and 5

Step 2 of Algorithms 1, 3, 4, and 5 require to localize a jump in the trajectory  $(\mathcal{C}_{\widehat{m}(C)})_{C \geq 0}$ , given the path  $(\widehat{m}(C))_{C \geq 0}$  and some complexity measure  $(\mathcal{C}_m)_{m \in \mathcal{M}}$ . Although the maximal jump is straightforward to localize, Theorem 1 suggests to look for the largest jump over a geometrical window of values of  $C$ , that is,  $\widehat{C}_{\text{window}}$  as defined by Eq. (19) in Section 2.5. This section explains how  $\widehat{C}_{\text{window}}$  can be computed efficiently given the path  $(\mathcal{C}_{\widehat{m}(C)})_{C \geq 0}$ , with a complexity  $\mathcal{O}(i_{\max} \log i_{\max}) = \mathcal{O}(\text{card } \mathcal{M} \log(\text{card } \mathcal{M}))$ .

Let us consider a slightly more general problem: given some  $\alpha > \beta > 0$ , compute

$$\widehat{\mathcal{C}}_{\text{window}}^{\text{gal}} := \operatorname{argmax}_{C \geq 0} \{ \mathcal{C}_{\widehat{m}(\beta C)} - \mathcal{C}_{\widehat{m}(\alpha C)} \}. \quad (105)$$

Note that  $\widehat{\mathcal{C}}_{\text{window}}^{\text{gal}}$  is usually not reduced to a singleton, but can be an interval or a finite union of intervals.

From Eq. (96) in Appendix B.1, the path  $(\mathcal{C}_{\widehat{m}(C)})_{C \geq 0}$  is piecewise constant and can be fully described with a small number of parameters: writing  $\mathcal{C}_i = \mathcal{C}_{m_i}$ ,

$$\forall i \in \{0, \dots, i_{\max}\}, \quad \forall C \in [C_i, C_{i+1}), \quad \mathcal{C}_{\widehat{m}(C)} = \mathcal{C}_i. \quad (106)$$

Given this description of  $(\mathcal{C}_{\widehat{m}(C)})_{C \geq 0}$ , Algorithm 8 below determines the set  $\widehat{\mathcal{C}}_{\text{window}}^{\text{gal}}$ , as proved by Proposition 6.

**Algorithm 8.** Input:  $(C_i)_{0 \leq i \leq i_{\max}+1}$  an increasing sequence of non-negative reals with  $C_0 = 0$  and  $C_{i_{\max}+1} = +\infty$ , and  $(\mathcal{C}_i)_{0 \leq i \leq i_{\max}}$  a sequence of real numbers.

1. If  $i_{\max} = 0$ , define  $\widehat{\mathcal{C}}_{\text{window}}^{\text{gal}} := [0, +\infty)$  and stop.

2. Otherwise, proceed and compute  $\bar{C} = (C_1/\beta, \dots, C_{i_{\max}}/\beta, C_1/\alpha, \dots, C_{i_{\max}}/\alpha) \in \mathbb{R}^{2i_{\max}}$  and  $\bar{\Delta} = (\mathcal{C}_1 - \mathcal{C}_0, \dots, \mathcal{C}_{i_{\max}} - \mathcal{C}_{i_{\max}-1}, \mathcal{C}_0 - \mathcal{C}_1, \dots, \mathcal{C}_{i_{\max}-1} - \mathcal{C}_{i_{\max}}) \in \mathbb{R}^{2i_{\max}}$ .
3. Sort  $\bar{C}$  and  $\bar{\Delta}$  according to  $\bar{C}$ , that is, find some permutation  $\sigma$  of  $\{1, \dots, 2i_{\max}\}$  such that  $\bar{C}_{\sigma(1)} \leq \dots \leq \bar{C}_{\sigma(2i_{\max})}$  and compute  $\bar{C}^\sigma = (\bar{C}_{\sigma(i)})_{1 \leq i \leq 2i_{\max}}$  and  $\bar{\Delta}^\sigma = (\bar{\Delta}_{\sigma(i)})_{1 \leq i \leq 2i_{\max}}$ .
4. Compute  $W := \text{cumsum}(\bar{\Delta}^\sigma) \in \mathbb{R}^{2i_{\max}}$ , that is, for every  $i \in \{1, \dots, 2i_{\max}\}$ ,

$$W_i = \sum_{j=1}^i \bar{\Delta}_j^\sigma.$$

5. Compute  $V \in \mathbb{R}^{2i_{\max}}$  such that, for every  $i \in \{1, \dots, 2i_{\max}\}$ ,  $V_i = W_i$  if  $\bar{C}_i^\sigma < \bar{C}_{i+1}^\sigma$ , and otherwise  $V_i = -\infty$ .
6. Determine  $\mathcal{K} := \text{argmax}_{i \in \{1, \dots, 2i_{\max}\}} V_i$ .
7. Define  $\widehat{\mathcal{E}}_{\text{window}}^{\text{gal}} := \bigcup_{k \in \mathcal{K}} [\bar{C}_k^\sigma, \bar{C}_{k+1}^\sigma)$  with  $\bar{C}_{2i_{\max}+1}^\sigma = +\infty$ .

Output:  $\widehat{\mathcal{E}}_{\text{window}}^{\text{gal}}$ .

**Proposition 6** (Correctness of Algorithm 8). *Algorithm 8 is correct, that is, it terminates and its output  $\widehat{\mathcal{E}}_{\text{window}}^{\text{gal}}$  actually satisfies Eq. (105) provided Eq. (106) holds true.*

*Proof of Proposition 6.* If  $i_{\max} = 0$ ,  $C \mapsto \mathcal{E}_{\widehat{m}(C)}$  is constant over  $[0, +\infty)$  so Algorithm 8 is correct. Otherwise, Eq. (106) can be rewritten as

$$\forall C \geq 0, \quad \mathcal{E}_{\widehat{m}(C)} = \mathcal{C}_0 + \sum_{i=1}^{i_{\max}} (\mathcal{C}_i - \mathcal{C}_{i-1}) \mathbb{1}_{C \geq \mathcal{C}_i}$$

hence, for every  $C \geq 0$ , using the notation of Algorithm 8,

$$\begin{aligned} \mathcal{E}_{\widehat{m}(\beta C)} - \mathcal{E}_{\widehat{m}(\alpha C)} &= \sum_{i=1}^{i_{\max}} (\mathcal{C}_i - \mathcal{C}_{i-1}) \mathbb{1}_{\beta C \geq \mathcal{C}_i} - \sum_{i=1}^{i_{\max}} (\mathcal{C}_i - \mathcal{C}_{i-1}) \mathbb{1}_{\alpha C \geq \mathcal{C}_i} \\ &= \sum_{i=1}^{2i_{\max}} \bar{\Delta}_i \mathbb{1}_{C \geq \bar{C}_i} = \sum_{i=1}^{2i_{\max}} \bar{\Delta}_i^\sigma \mathbb{1}_{C \geq \bar{C}_i^\sigma} = \sum_{i=1}^{2i_{\max}} W_i \mathbb{1}_{C \in [\bar{C}_i^\sigma, \bar{C}_{i+1}^\sigma)} \\ &= \sum_{i=1}^{2i_{\max}} V_i \mathbb{1}_{C \in [\bar{C}_i^\sigma, \bar{C}_{i+1}^\sigma)} \end{aligned} \quad (107)$$

with the conventions  $\bar{C}_{2i_{\max}+1}^\sigma = +\infty$  and  $\infty \mathbb{1}_{C \in \emptyset} = 0$ . For the last equality, we use the fact that when  $[\bar{C}_i^\sigma, \bar{C}_{i+1}^\sigma)$  is empty —which corresponds to values of  $\bar{C}_i^\sigma$  that are equal to  $C_j/\beta = C_k/\alpha$  for some  $j, k \in \{1, \dots, i_{\max}\}$ —, the value of  $W_i \mathbb{1}_{C \in [\bar{C}_i^\sigma, \bar{C}_{i+1}^\sigma)}$  is zero whatever  $W_i$ , hence  $W_i$  can be changed into  $V_i$ .

By Eq. (107),

$$\sup_{C \geq 0} \{ \mathcal{E}_{\widehat{m}(\beta C)} - \mathcal{E}_{\widehat{m}(\alpha C)} \} = \max_{1 \leq i \leq 2i_{\max}} V_i$$

and the supremum is attained exactly at the values of  $C$  belonging to some interval  $[\bar{C}_k^\sigma, \bar{C}_{k+1}^\sigma)$  with  $k \in \mathcal{K} = \text{argmax}_i V_i$ . In other words, Algorithm 8 is correct.  $\square$

## Appendix C: More figures and experimental results

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File: survey\_penmin.tex, compiled with jsfds, version : 2018/06/13

date: October 23, 2019

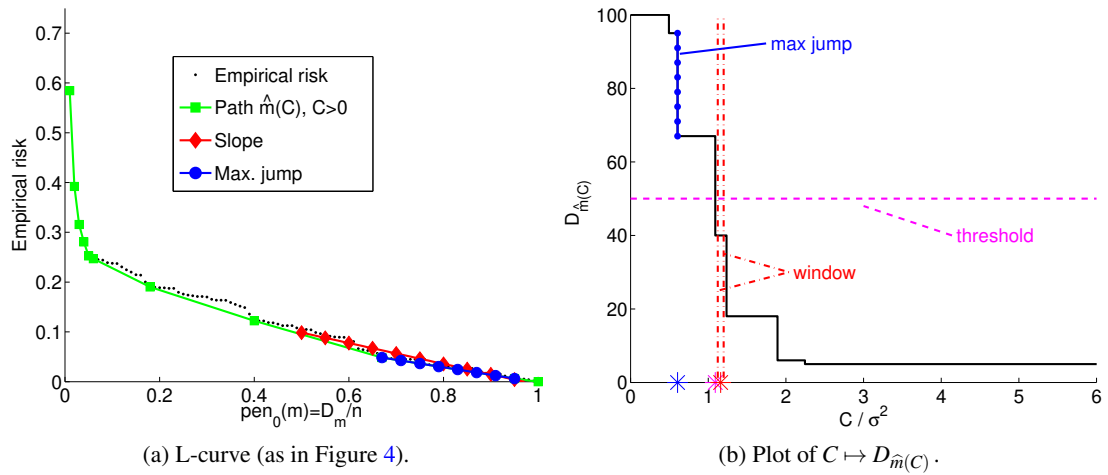


FIGURE 9. On the same sample, visualization of the three versions of Algorithm 1 and of  $\hat{C}_{\text{slope}}$ . ‘Easy’ setting, see Appendix D for details.

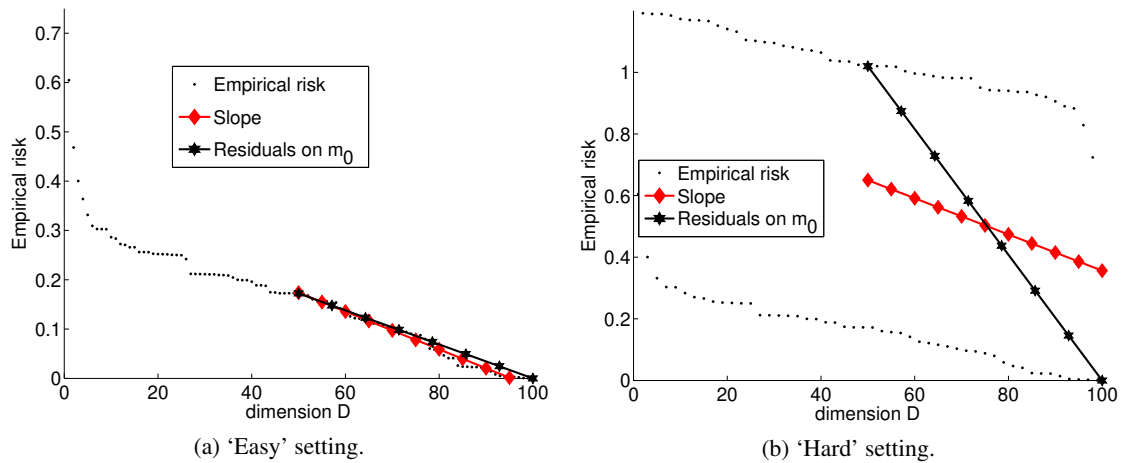


FIGURE 10. Slope estimation  $\hat{C}_{\text{slope}}$  vs. residual-based variance estimator  $\hat{\sigma}_{m_0}^2$ . See Appendix D for details.

$\widehat{C}$	$\mathbb{E}[\widehat{C}/\sigma^2]$	$\sqrt{\text{var}(\widehat{C})}/\sigma^2$	$\mathbb{E}[(\widehat{C} - \sigma^2)^2]/\sigma^4$	risk ratio
$\widehat{C}_{\text{maxj.}}$	1.09	0.257	0.0749	$1.309 \pm 0.003$
$\widehat{C}_{\text{thr.}}, T_n = n/10$	3.12	1.281	6.140	$1.647 \pm 0.004$
$\widehat{C}_{\text{thr.}}, T_n = n/\log(n)$	1.60	0.469	0.584	$1.310 \pm 0.002$
$\widehat{C}_{\text{thr.}}, \mathbf{T}_n = \mathbf{n}/2$	1.13	0.229	0.0683	$1.278 \pm 0.003$
$\widehat{C}_{\text{thr.}}, T_n = 9n/10$	0.84	0.239	0.0826	$1.621 \pm 0.083$
$\widehat{C}_{\text{window}}, \eta = 1/n$	1.09	0.257	0.0745	$1.309 \pm 0.003$
$\widehat{C}_{\text{window}}, \eta = \mathbf{1}/\sqrt{\mathbf{n}}$	1.10	0.256	0.0752	$1.308 \pm 0.003$
$\widehat{C}_{\text{window}}, \eta = 1.5/\sqrt{n}$	1.10	0.258	0.0776	$1.307 \pm 0.003$
$\widehat{C}_{\text{window}}, \eta = \sqrt{\log(n)/n}$	1.12	0.263	0.0829	$1.304 \pm 0.003$
$\widehat{C}_{\text{window}}, \eta = 2\sqrt{\log(n)/n}$	1.17	0.286	0.110	$1.294 \pm 0.003$
$\widehat{C}_{\text{slope}}, D_0 = n/10$	1.15	0.181	0.0544	$1.243 \pm 0.002$
$\widehat{C}_{\text{slope}}, D_0 = n/\log(n)$	1.09	0.188	0.0437	$1.260 \pm 0.002$
$\widehat{C}_{\text{slope}}, \mathbf{D}_0 = \mathbf{n}/2$	1.05	0.228	0.0543	$1.313 \pm 0.003$
$\widehat{C}_{\text{slope}}, D_0 = 9n/10$	1.02	0.478	0.229	$1.672 \pm 0.009$
CAPUSHE	1.05	0.291	0.0873	$1.410 \pm 0.005$
median	1.08	0.229	0.0588	$1.301 \pm 0.003$
consensus	–	–	–	$1.306 \pm 0.003$
consensus when no reject	–	–	–	$1.298 \pm 0.003$
$\widehat{\sigma}_{m_0}^2, D_{m_0} = n/10$	1.23	0.180	0.0862	$1.237 \pm 0.002$
$\widehat{\sigma}_{m_0}^2, D_{m_0} = n/\log(n)$	1.12	0.176	0.0443	$1.241 \pm 0.002$
$\widehat{\sigma}_{m_0}^2, D_{m_0} = n/2$	1.05	0.211	0.0469	$1.304 \pm 0.003$
$\widehat{\sigma}_{m_0}^2, D_{m_0} = n/2 + 1$	1.05	0.213	0.0478	$1.305 \pm 0.003$
$\widehat{\sigma}_{m_0}^2, D_{m_0} = 9n/10$	1.02	0.455	0.2080	$1.641 \pm 0.008$
$C_p$ (known $\sigma^2$ )	–	–	–	$1.269 \pm 0.003$
$C_p \times 1.12$ (known $\sigma^2$ )	–	–	–	$1.251 \pm 0.002$

TABLE 2. Algorithms 1–2, ‘easy’ setting: distribution of  $\widehat{C}$  and model-selection performance, with various definitions for  $\widehat{C}$  and various parameters for each definition. The risk ratio is  $\mathbb{E}[\|\widehat{F}_{\widehat{m}} - F\|^2 / \inf_{m \in \mathcal{M}} \|\widehat{F}_m - F\|^2]$ . Reported values are empirical estimates obtained from  $N = 10000$  independent samples. For the risk ratio, error bars are equal to the standard deviation of the ratio  $\|\widehat{F}_{\widehat{m}} - F\|^2 / \inf_{m \in \mathcal{M}} \|\widehat{F}_m - F\|^2$  divided by  $\sqrt{N}$ .

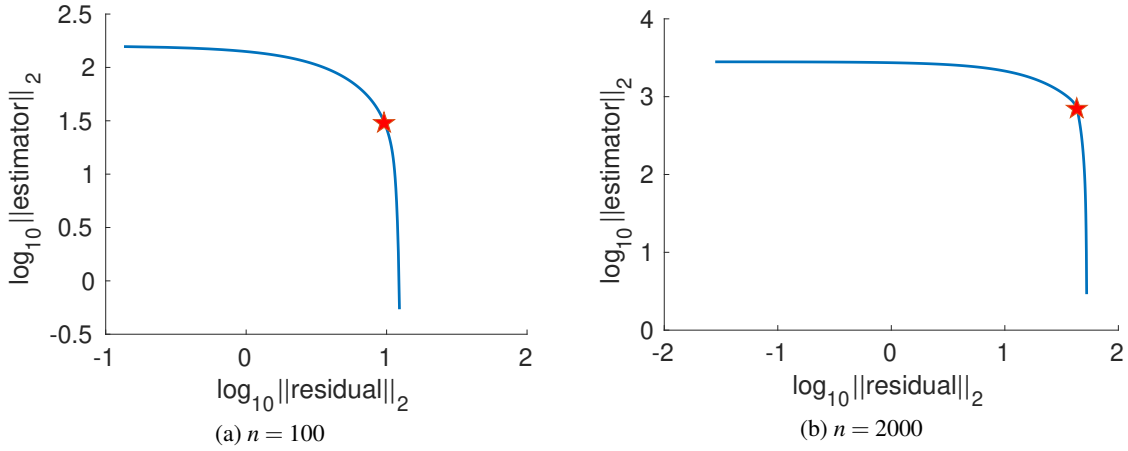


FIGURE 11.  $L$ -curve  $(\log_{10}\|Y - \hat{F}_\lambda\|, \log_{10}\|\hat{F}_\lambda\|)_{\lambda>0}$  in the ‘kernel ridge’ framework. See Appendix D for details. The red star shows the position of the oracle (minimum of the risk  $n^{-1}\|F - \hat{F}_\lambda\|^2$ ). The “elbow” is clearly localized for  $n = 2000$  (and close to the oracle), but not for  $n = 100$ .

$\hat{C}$	$\mathbb{E}[\hat{C}/\sigma^2]$	$\sqrt{\text{var}(\hat{C})}/\sigma^2$	$\mathbb{E}[(\hat{C} - \sigma^2)^2]/\sigma^4$	risk ratio
$\hat{C}_{\text{maxj.}}$	1.10	0.259	0.076	$1.291 \pm 0.003$
$\hat{C}_{\text{thr.}, T_n = n/10}$	3.38	1.390	7.57	$1.661 \pm 0.004$
$\hat{C}_{\text{thr.}, T_n = n/\log(n)}$	1.59	0.462	0.563	$1.285 \pm 0.002$
$\hat{C}_{\text{thr.}, \mathbf{T}_n = \mathbf{n}/2}$	1.13	0.231	0.0703	$1.258 \pm 0.002$
$\hat{C}_{\text{thr.}, T_n = 9n/10}$	0.86	0.236	0.077	$1.566 \pm 0.008$
$\hat{C}_{\text{window}, \eta = 1/n}$	1.09	0.257	0.0746	$1.292 \pm 0.003$
$\hat{C}_{\text{window}, \eta = 1/\sqrt{n}}$	1.10	0.257	0.0762	$1.288 \pm 0.003$
$\hat{C}_{\text{window}, \eta = 1.5/\sqrt{n}}$	1.11	0.258	0.078	$1.288 \pm 0.003$
$\hat{C}_{\text{window}, \eta = \sqrt{\log(n)/n}}$	1.12	0.263	0.0827	$1.287 \pm 0.003$
$\hat{C}_{\text{window}, \eta = 2\sqrt{\log(n)/n}}$	1.17	0.285	0.109	$1.275 \pm 0.003$
$\hat{C}_{\text{slope}, D_0 = n/10}$	1.54	0.188	0.328	$1.268 \pm 0.002$
$\hat{C}_{\text{slope}, D_0 = n/\log(n)}$	1.65	0.193	0.46	$1.291 \pm 0.002$
$\hat{C}_{\text{slope}, \mathbf{D}_0 = \mathbf{n}/2}$	2.36	0.231	1.89	$1.437 \pm 0.003$
$\hat{C}_{\text{slope}, D_0 = 9n/10}$	20.2	2.07	374	$3.68 \pm 0.016$
CAPUSHE	2.77	1.66	5.87	$1.562 \pm 0.005$
median	1.16	0.253	0.0911	$1.260 \pm 0.002$
consensus	–	–	–	$1.285 \pm 0.003$
consensus when no reject	–	–	–	$1.266 \pm 0.003$
$\hat{\sigma}_{m_0}^2, D_{m_0} = n/10$	5.44	0.473	19.9	$2.055 \pm 0.006$
$\hat{\sigma}_{m_0}^2, D_{m_0} = n/\log(n)$	1.12	0.176	0.0443	$1.223 \pm 0.002$
$\hat{\sigma}_{m_0}^2, D_{m_0} = n/2$	8.94	0.828	63.7	$2.577 \pm 0.006$
$\hat{\sigma}_{m_0}^2, D_{m_0} = n/2 + 1$	1.05	0.213	0.0478	$1.285 \pm 0.003$
$\hat{\sigma}_{m_0}^2, D_{m_0} = 9n/10$	38.9	3.95	1450	$6.11 \pm 0.011$
$C_p$ (known $\sigma^2$ )	–	–	–	$1.252 \pm 0.003$
$C_p \times 1.12$ (known $\sigma^2$ )	–	–	–	$1.232 \pm 0.002$

TABLE 3. Same as Table 2 for the ‘hard’ setting.

## Appendix D: Detailed information about figures and simulation experiments

This section provides all details necessary to reproduce the figures and simulation experiments reported throughout the article.

### D.1. Data and estimators

All experiments are made within the fixed-design regression framework described in Section 2.1, with two main kinds of estimator collections and data.

**Least-squares framework (‘easy’/‘hard’)** All figures and tables, except Figures 3 and 11, consider data and estimators as follows. Data satisfy

$$Y = F + \varepsilon \in \mathbb{R}^n$$

with independent Gaussian noise  $\varepsilon \sim \mathcal{N}(0, \sigma^2 I_n)$ ,  $\sigma^2 = 1/4$ ,  $n = 100$ ,

$$F_i = \frac{C_n}{i} \quad \text{and} \quad C_n = \left( \sum_{i=1}^n \frac{1}{i^2} \right)^{-1/2}.$$

The choice of  $C_n$  ensures that  $n^{-1} \|F\|^2 = 1$ .

The estimators considered are least-squares (projection) estimators with one among the following two collections of models  $(S_m)_{1 \leq m \leq n}$ :

- ‘easy’ setting: for every  $m \in \{1, \dots, n\}$ ,  $S_m = S_m^{\text{easy}}$  is the linear span of the first  $m$  vectors of the canonical basis of  $\mathbb{R}^n$ .
- ‘hard’ setting: for every  $m \in \{1, \dots, n\}$ ,  $S_m = S_m^{\text{hard}}$  is the linear span of the first  $m$  vectors of the canonical basis of  $\mathbb{R}^n$  if  $m$  is odd, and  $S_m = S_m^{\text{hard}}$  is the linear span of the last  $m$  vectors of the canonical basis of  $\mathbb{R}^n$  if  $m$  is even.

Both settings correspond to (ordered) variable selection with an orthogonal design, after having transformed the data conveniently according to the design matrix. In the easy case, the variables are ordered by decreasing order of magnitude. In the hard case, some uncertainty remains about the correct order (ascending or descending), and the two options are considered alternatively (depending on the parity of  $n$ ). Of course, models  $S_m^{\text{hard}}$  with  $m$  even are very poor, but this can be unknown before seeing the data.

**Kernel ridge framework** Figures 3 and 11 consider data and estimators as follows. Data satisfy

$$Y = F + \varepsilon \in \mathbb{R}^n$$

with independent Gaussian noise  $\varepsilon \sim \mathcal{N}(0, \sigma^2 I_n)$ ,  $\sigma^2 = 1$ ,

$$F_1 = \frac{1}{2} \quad \text{and} \quad \forall i \in \{2, \dots, n\}, \quad F_i = \sin(25\pi x_i^3) \quad \text{with} \quad x_i = \frac{i-1}{n-1}.$$

The family of estimators considered is the family of kernel ridge estimators  $(\hat{F}_\lambda)_{\lambda > 0}$  where for every  $\lambda > 0$ ,

$$\hat{F}_\lambda = K(K + n\lambda I_n)^{-1}Y, \quad K = (k(x_i, x_j))_{1 \leq i, j \leq n}, \quad \text{and} \quad \forall x, x' \in \mathbb{R}, k(x, x') = \exp(-\alpha|x - x'|)$$



the Laplace kernel, with  $\alpha = 8$ . In the experiments, only a finite set  $\{\lambda_0, \dots, \lambda_n\}$  of values of  $\lambda$  is considered, chosen such that the degrees of freedom  $\text{tr}(K(K + n\lambda_i I_n)^{-1})$  are equal to  $i$  for every  $i = 0, \dots, n$ .

## D.2. Procedures

The exact definitions of all procedures considered in the experiments for computing some  $\hat{C}$  or choosing some model  $\hat{m}$  are the following. For the procedures depending on some parameter, its default value is used everywhere except in Tables 2–3. Note that the choice of the default values was made *prior to the simulations*: we can check afterwards on Tables 2–3 that these choices provide reasonably good results (which fortunately happened), so that results using only the default values of the parameters (for instance, Table 1) are meaningful.

**Maximal jump** ( $\hat{C}_{\text{max.j.}}$ , ‘Max. jump’, ‘max j.’ or ‘max’) In Section 7.1, we define

$$\hat{C}_{\text{max.j.}} \in \operatorname{argmax}_{C \geq 0} \left\{ D_{\hat{m}_{\min}^{(0)}(C^-)} - D_{\hat{m}_{\min}^{(0)}(C^+)} \right\},$$

that is, the location of the maximal jump of  $C \mapsto D_{\hat{m}_{\min}^{(0)}(C)}$ , assuming it is unique. In our experiments, when the  $\operatorname{argmax}$  contains several values of  $C$ , we choose the largest one, that is, the last largest jump; this choice is natural, since it means taking the less complex model among those corresponding to a maximal jump, and it matches the choice made by [Lerasle and Takahashi \(2011\)](#).

Note that for change-point detection, [Lebarbier \(2005, Section 4.2\)](#) suggests an opposite convention —taking the smallest value of  $C$  in the  $\operatorname{argmax}$ —, arguing from simulation experiments that otherwise too small models are selected. Nevertheless, [Lebarbier \(2005, Section 4.2\)](#) also reports that the latter convention can lead to taking  $\hat{C}_{\text{max.j.}}$  too small, so a rather complicated method is suggested for choosing some threshold  $\alpha_{\text{thr}}$  and imposing  $\hat{C}_{\text{max.j.}} \geq \alpha_{\text{thr}}$ .

**Threshold** ( $\hat{C}_{\text{thr.}}$  or ‘thr’) Eq. (20) in Section 2.5 defines

$$\hat{C}_{\text{thr.}}(T_n) := \min \{ C \geq 0 / D_{\hat{m}(C)} \leq T_n \},$$

which depends on some parameter  $T_n$ . The default value of  $T_n$  is  $n/2$ .

Note that Theorem 1 suggests that  $T_n = \rho n$  works for any  $\rho \in (0, 1)$ , and previous theoretical results ([Arlot and Massart, 2009, Section 3.3](#)) suggest to take  $T_n \propto n/\log(n)$  or  $n/(\log n)^2$ . Nevertheless, all these theoretical results involve pessimistic constants (as shown by the simulation experiments), so they cannot be used for a fine tuning of  $T_n$ . It turns out that  $n/2$  does very good in the experiments of Tables 2–3, while other choices lead to much worse performance.

**Window** ( $\hat{C}_{\text{window}}$  or ‘win’) Eq. (19) in Section 2.5 defines

$$\hat{C}_{\text{window}}(\eta) \in \operatorname{argmax}_{C \geq 0} \left\{ D_{\hat{m}(C/[1+\eta])} - D_{\hat{m}(C[1+\eta])} \right\},$$

which depends on some parameter  $\eta > 0$ . Similarly to  $\hat{C}_{\text{max.j.}}$ , the  $\operatorname{argmax}$  is usually not reduced to a single point, so a more precise definition must be given for  $\hat{C}_{\text{window}}$ . Actually, when  $\eta > 0$ ,

Appendix B.2 shows that  $\operatorname{argmax}_{C \geq 0} \{D_{\widehat{m}(C/[1+\eta])} - D_{\widehat{m}(C[1+\eta])}\}$  is a finite union of intervals. Denoting by  $[\widehat{C}_{\text{window}}^{(1)}, \widehat{C}_{\text{window}}^{(2)})$  the last of these intervals—that is, the one corresponding to the largest values of  $C$ —we define

$$\widehat{C}_{\text{window}} = \sqrt{\widehat{C}_{\text{window}}^{(1)} \widehat{C}_{\text{window}}^{(2)}}.$$

Of course, other choices could be possible and we do not claim that our (arbitrary) choice is the best one.

In Figures 5 and 9b, the interval represented by the two red vertical lines is  $[\widehat{C}_{\text{window}}^{(1)}, \widehat{C}_{\text{window}}^{(2)})$ . Note that this interval often looks like  $[\widehat{C}_{\text{window}}/(1+\eta), \widehat{C}_{\text{window}}(1+\eta))$  but it can also be quite different.

Taking the limit  $\eta \rightarrow 0^+$  in the definition of  $\widehat{C}_{\text{window}}$ , we recover  $\widehat{C}_{\text{maxj}}$ . Theorem 1 suggests to take  $\eta \propto \eta_n^+ \geq \sqrt{\log(n)/n}$ , that we consider in our experiments (see Tables 2–3). In our experiments, the default value for  $\eta$  is  $n^{-1/2}$ , a choice made to get a slightly smaller value than  $\sqrt{\log(n)/n} \approx 0.22$  (we recall that  $n = 100$  in the least-squares framework).

**Slope ( $\widehat{C}_{\text{slope}}$  or ‘slope’)** In Algorithm 2, the definition of  $\widehat{C}_{\text{slope}}$  is rather vague; it is a bit more precise in Section 7 where the range of models considered in the regression is defined by  $\text{pen}_0(m) \in [p_{\min}, p_{\max}]$  for some  $p_{\min} < p_{\max}$  to be chosen. In the experiments, since  $\text{pen}_0(m)$  is equal to  $D_m/n$  in the least-squares framework, we choose  $p_{\min} = D_0/n$  and  $p_{\max} = 1$  for some parameter  $D_0 \in [1, n)$ .

In other words, given  $D_0 \in [1, n)$ , we consider only models of dimension  $D_m \geq D_0$  and we perform a (standard) linear regression of the empirical risk  $n^{-1} \|\widehat{F}_m - F\|^2$  against  $-D_m/n$ , that is, we solve

$$(\widehat{a}, \widehat{b}) \in \operatorname{argmin}_{(a,b) \in \mathbb{R}^2} \sum_{m \in \mathcal{M} / D_m \geq D_0} \left( a - b \frac{D_m}{n} - \frac{1}{n} \|\widehat{F}_m - F\|^2 \right)^2,$$

and we define  $\widehat{C}_{\text{slope}}$  as the resulting slope  $\widehat{b}$ . The default value of  $D_0$  is  $n/2$ .

**Capushe ( $\widehat{C}_{\text{CAPUSHE}}, \widehat{m}_{\text{CAPUSHE}}$  or ‘CAP’)** The procedure called ‘CAPUSHE’ throughout this article is the one proposed by Baudry et al. (2012, Section 4.2) and implemented in the CAPUSHE package for Matlab and R. For completeness, let us recall its definition—which depends on some parameter  $pct \in (0, 1)$ —in the least-squares framework.

- Step 1: If several models have the same dimension  $D$ , keep only the one with the smallest empirical risk. This step does not change anything in our experimental setting since there is exactly one model per dimension.
- Step 2: for all  $D \in [1, n-2]$ , compute by robust linear regression the slope  $\widehat{C}_s(D)$  of the empirical risk  $n^{-1} \|\widehat{F}_m - F\|^2$  against  $-D_m/n$ , among models of dimension  $D_m \geq D$ .
- Step 3: for all  $D \in [1, n-2]$ , compute the corresponding selected model

$$\widehat{m}_D = \widehat{m}(2\widehat{C}_s(D)) = \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \frac{1}{n} \|\widehat{F}_m - Y\|^2 + \frac{2\widehat{C}_s(D)D_m}{n} \right\}.$$

Then,  $\widehat{m}_1, \dots, \widehat{m}_{n-2}$  is piecewise constant, and some  $1 = D_1 < \dots < D_{I+1} = n - 1$  and  $m_1, \dots, m_{I+1} \in \mathcal{M}$  exist such that

$$\forall i \in \{1, \dots, I\}, \forall D \in [D_i, D_{i+1} - 1], \quad \widehat{m}_D = m_i$$

with  $m_1 \neq m_2, \dots, m_I \neq m_{I+1}$ . The intervals  $[D_i, D_{i+1} - 1]$  are called ‘‘plateau’’ (platforms) by [Baudry et al. \(2012, Section 4.2\)](#) and their size is denoted by  $N_i = D_{i+1} - D_i$ .

- Step 4: Keep only the platforms of size  $N_i$  larger than  $pct$  times the total size  $\sum_\ell N_\ell = n - 2$ , and among these, define  $\widehat{i}$  the last platform, that is,

$$\widehat{i} = \max \left\{ i \in \{1, \dots, I\} / N_i > pct \times (n - 2) \right\}$$

and select

$$\widehat{m}_{\text{CAPUSHE}} = m_{\widehat{i}}.$$

Note that at step 4, it can happen that no platform is large enough. In such cases, we consider the last platform among the ones of largest size, that is,

$$\widehat{i} = \max \left\{ i \in \{1, \dots, I\} / N_i = \max_j N_j \right\}.$$

We always take  $pct = 0.15$  in our experiments, that is, the default value proposed by [Baudry et al. \(2012\)](#).

Note that [Baudry et al. \(2012\)](#) only provide a model-selection procedure  $\widehat{m}_{\text{CAPUSHE}}$ , and not a value  $\widehat{C}$  of the constant in front of the penalty. In order to help understanding better  $\widehat{m}_{\text{CAPUSHE}}$ , we also report in our experiments the distribution of  $\widehat{C}_{\text{CAPUSHE}}$  that we define as some median of

$$\left\{ \widehat{C}_s(D_{\widehat{i}}), \dots, \widehat{C}_s(D_{\widehat{i}+1} - 1) \right\}.$$

This choice is arbitrary among many others that all lead to having  $\widehat{m}_{\text{CAPUSHE}} = \widehat{m}(2\widehat{C}_{\text{CAPUSHE}})$ .

**Median (‘med’)** As defined in the caption of [Figure 6](#), ‘median’ refers to taking  $\widehat{C}$  as the median of

$$\left\{ \widehat{C}_{\text{max.j.}}, \widehat{C}_{\text{thr.}}, \widehat{C}_{\text{window}}, \widehat{C}_{\text{slope}}, \widehat{C}_{\text{CAPUSHE}} \right\}$$

(with their default parameter values for  $\widehat{C}_{\text{thr.}}$ ,  $\widehat{C}_{\text{window}}$ , and  $\widehat{C}_{\text{slope}}$ :  $T_n = n/2$ ,  $\eta = n^{-1/2}$ ,  $D_0 = n/2$ ), and  $\widehat{m} = \widehat{m}(2\widehat{C})$ .

Remark that the set of procedures considered is arbitrary, and other choices could be made. Nevertheless, it seems wise to keep an equilibrium between the jump and slope formulations; here, the jump approach is slightly favored, but the slope definitions come into play when  $\widehat{C}_{\text{max.j.}}$ ,  $\widehat{C}_{\text{thr.}}$ , and  $\widehat{C}_{\text{window}}$  do not exactly coincide.

The idea of considering some median of several values of  $\widehat{C}$  could also be used when there is some uncertainty about the parameter of some procedure (say,  $T_n$  for  $\widehat{C}_{\text{thr.}}$ ), by considering the median of the set of values obtained on a grid of values of the parameter.

**Residuals** ( $\widehat{\sigma}_{m_0}^2$ , ‘Residuals on  $m_0$ ’ or ‘resid’) The residual-based variance estimator  $\widehat{\sigma}_{m_0}^2$  is defined by Eq. (71) in Section 6.1:

$$\widehat{\sigma}_{m_0}^2 := \frac{1}{n - D_{m_0}} \left\| Y - \widehat{F}_{m_0} \right\|^2$$

for some model  $m_0$ . In the experiments, there is one model per dimension, so  $m_0$  is given by the value of its dimension  $D_{m_0}$  and the default choice is  $D_{m_0} = n/2$ . Since  $n = 100$ , the default choice is  $D_{m_0} = 50$  which is even, so the definition of  $S_m^{\text{hard}}$ —in which models of odd dimension are good and models of even dimension are very poor—is made on purpose.

Note that in Tables 2–3, the line “ $D_{m_0} = n/\log(n)$ ” means “ $D_{m_0} = 21$ ” (hence, for the ‘hard’ setting, it is a reasonably good model).

**Consensus** (‘cons’) As defined in the caption of Figure 7, the “consensus” procedure performs a majority vote among

$$\left\{ \widehat{m}(2\widehat{C}_{\text{max.j.}}), \widehat{m}(2\widehat{C}_{\text{thr.}}), \widehat{m}(2\widehat{C}_{\text{window}}), \widehat{m}(2\widehat{C}_{\text{slope}}), \widehat{m}_{\text{CAPUSHE}} \right\}$$

with their default parameters values. If no majority emerges (that is, if we do not have at least three of these procedures that agree), the default choice is  $\widehat{m}(2\widehat{C}_{\text{window}})$ . Remark that Table 1 shows that an agreement occurs for more than 96% of the samples in the ‘easy’ setting, and for more than 89% of the samples in the ‘hard’ setting.

**Consensus when no reject** (‘no rej’) This actually refers to the same procedure as ‘consensus’, but showing results (a boxplot or an estimation of the expectation of the loss ratio) only for the samples for which a majority emerged. Again, Table 1 shows that this only removes a small fraction of the  $N = 10^4$  independent samples generated in our experiments.

**Mallows’  $C_p$**  When the variance  $\sigma^2$  is known, a natural model-selection procedure for the framework of Section 2 is Mallows’  $C_p$  (Mallows, 1973), that is, selecting

$$\widehat{m} = \widehat{m}(2\sigma^2) = \operatorname{argmin}_{m \in \mathcal{M}} \left\{ \frac{1}{n} \left\| \widehat{F}_m - Y \right\|^2 + \frac{2\sigma^2 D_m}{n} \right\}.$$

Its performance is shown in Tables 2–3 for comparison.

Mallows’  $C_p$  is also considered for illustrating the overpenalization phenomenon in Figure 8 in Section 8.4. On the graph of Figure 8, what is plotted is, for  $C \in [0, 4]$ , the estimated value (from  $N = 10^4$  independent samples) of the expected risk ratio

$$\mathbb{E} \left[ \frac{\left\| \widehat{F}_{\widehat{m}(2C\sigma^2)} - F \right\|^2}{\inf_{m \in \mathcal{M}} \left\| \widehat{F}_m - F \right\|^2} \right]$$

when using Mallows’  $C_p$  penalty multiplied by  $C$ ; we recall that  $\widehat{m}(\cdot)$  is defined by Eq. (10) in Section 2.3. For plotting the graph of Figure 8, a linear grid of values of  $C$  with stepsize 1/100 is considered. The optimal performance is obtained for  $C = 1.12$  in the ‘easy’ and ‘hard’ settings, and it is also included in Tables 2–3.

### ***D.3. Additional remarks***

Repeated experiments show results obtained from  $N = 10^4$  independent samples.

Illustrations made on a single sample in the least-squares framework are showed in Figures 2, 4, 5, 9, 10. The samples considered have been chosen manually in order to illustrate either typical or rare (but still possible) configurations. The graphs of Figure 2, Figure 4, and Figure 10a are made on the same sample (they correspond to a “typical” situation). The graph of Figure 5 is made on a second sample (corresponding to a “rare” situation). The two graphs of Figure 9 are made on a third sample (also corresponding to a “rare” situation, similar to the one shown in Figure 5).

Figure 3 is taken from the article by Arlot and Bach (2011, top right graph of Figure 2). It is made from a single sample generated as in the kernel-ridge framework (see Appendix D.1), with a sample size  $n = 200$ .