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A Threshold Regularization Method for Inverse Problems

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Abstract

A number of regularization methods for discrete inverse problems consist in considering weighted versions of the usual least square solution. However, these so-called filter methods are generally restricted to monotonic transformations, e.g. the Tikhonov regularization or the spectral cut-off. In this paper, we point out that in several cases, non-monotonic sequences of filters are more efficient. We study a regularization method that naturally extends the spectral cut-off procedure to non-monotonic sequences and provide several oracle inequalities, showing the method to be nearly optimal under mild assumptions. Then, we extend the method to inverse problems with noisy operator and provide efficiency results in a newly introduced conditional framework.

Keywords: Inverse problems; regularization; oracle inequalities; hard thresholding
Subject Class. MSC-2000 : 62G05, 62G08

1 Introduction

We are interested in recovering an unobservable signal x_0 , based on noisy observations of the image of x_0 through a linear operator A . The observation y satisfies the following relation

$$y(t) = Ax_0(t) + \varepsilon(t),$$

where $\varepsilon(\cdot)$ is a random process representing the noise. This problem is studied in [5], [12], [14] and in many applied fields such as medical imaging in [18] or seismography in [19] for instance. When the measured signal is only available at a finite number of points t_1, \dots, t_n ,

the operator A must be replaced by a discrete version $A_n : x \mapsto (Ax(t_1), \dots, Ax(t_n))'$, leading to a discrete linear model

$$y = A_n x_0 + \varepsilon,$$

with $y \in \mathbb{R}^n$. Difficulties in estimating x_0 occur when the problem is *ill-posed*, in the sense that small perturbations in the observations induce large changes in the solution. This is caused by an ill-conditioning of the operator A_n , reflected by a fast decay of its spectral values b_i . In such problems, the least square solution, although having a small bias, is generally inefficient due to a too large variance. Hence, *regularization* of the problem is required to improve the estimation. A large number of regularization methods are based on considering weighted versions of the least square estimator. The idea is to allocate low weights λ_i , or *filters*, to the least square coefficients that are highly contaminated with noise, thus reducing the variance, at the cost of increasing the bias at the same time. The most famous filter-based method is arguably the one due to Tikhonov (see [20]), where a collection of filters is indirectly obtained via a minimization procedure with ℓ^2 penalization. Tikhonov filters are entirely determined by a parameter τ that controls the balance between the minimization of the ℓ^2 norm of the estimator and the residual.

Another well spread filter method that will be given a particular interest in this paper, is the *spectral cut-off* discussed in [2], [9] and [11]. One simply considers a truncated version of the least square solution, where all coefficients corresponding to arbitrarily small eigenvalues are removed. Thus, spectral cut-off is associated to binary filters λ_i , equal to 1 if the corresponding eigenvalue b_i exceeds in absolute value a certain threshold τ , and 0 otherwise.

A common feature of spectral cut-off and Tikhonov regularization is the predetermined nature of the filters λ_i , defined in each case as a fixed non-decreasing function $f(\tau, \cdot)$ of the eigenvalues b_i^2 , and where only the parameter τ is allowed to depend on the observations. However, in many situations, non-monotonic sequences of filters may provide a more efficient estimation of x_0 . Actually, optimal values for λ_i generally depend on both the noise level, which is determined by the eigenvalue b_i , and the component, say x_i , of x_0 in the direction associated to b_i . A restriction to monotonic collections of filters turns out to be inefficient in situations where the coefficients x_i are uncorrelated to the spectral values b_i of the operator A_n .

Regularization methods involving more general classes of filters have also been treated in the literature. In [5], the authors study a general procedure known as *unbiased risk estimation*, that applies to arbitrary classes of filters, dealing in particular with non-monotonic collections. However, their general framework concerning the class of estimators requires in return additional regularity assumptions which we intend to relax in this paper. We focus on a specific class of projection estimators that extends the spectral cut-off to non-monotonic collections of filters. Precisely, we consider the collection of unrestricted binary filters $\lambda_i \in \{0, 1\}$. The computation of the estimator relies on the choice of a proper set of

coefficients $m \subset \{1, \dots, n\}$, which considerably increases the number of possibilities compared to the spectral cut-off procedure. We show this method to satisfy a non-asymptotic exact oracle inequality, when the oracle is computed in the class of binary filters. Moreover, we show our estimator to nearly achieve the rate of convergence of the best linear estimator in the maximal class of filters, i.e. when no restriction is made on λ_i .

In many actual situations, the operator A_n is not known precisely and only an approximation of it is available. Regularization of inverse problems with approximate operator is studied in [6], [8] and [13]. In this paper, we tackle the problem of estimating x_0 in the situation where we observe independently a noisy version \hat{b}_i of each eigenvalue b_i . We consider a new framework where the observations \hat{b}_i are made once and for all, and are seen as non-random. We provide a bound on the conditional risk of the estimator, given the values of \hat{b}_i , in the form of a conditional oracle inequality.

The paper is organized as follows. We introduce the problem in Section 2. We define our estimator in Section 3, and provide two types of oracle inequalities. Section 4 is devoted to an application of the method to inverse problems with noisy operators. The proofs of the results are postponed to the Appendix.

2 Problem setting

Let $(\mathcal{X}, \|\cdot\|)$ be a Hilbert space and $A_n : \mathcal{X} \rightarrow \mathbb{R}^n$ ($n > 2$) a linear operator. We want to recover an unknown signal $x_0 \in \mathcal{X}$ based on the indirect observations

$$y = A_n x_0 + \varepsilon, \tag{1}$$

where ε is a random noise vector. We assume that ε is centered with covariance matrix $\sigma^2 I$, where I denotes the identity matrix. We endow \mathbb{R}^n with the scalar product $\langle u, v \rangle_n = n^{-1} \sum_{i=1}^n u_i v_i$ and the associated norm $\|\cdot\|_n$ and we note $A_n^* : \mathbb{R}^n \rightarrow \mathcal{X}$ the adjoint of A_n . Let \mathcal{K}_n be the kernel of A_n and \mathcal{K}_n^\perp its orthogonal in \mathcal{X} which we assume to be of dimension n . The surjectivity of A_n ensures that the observation y provides information in all directions. If this condition is not met, one may simply reduce the dimension of the image in order to make A_n surjective.

The efficiency of the estimator relies first of all on the accuracy of the discrete operator A_n and how "close" it is to the true value A . The convergence of the estimator towards x_0 is subject to the condition that the distance of x_0 to the set \mathcal{K}_n^\perp tends to 0, which is reflected by a proper asymptotic behavior of the design t_1, \dots, t_n . This aspect is not discussed here, we consider a framework where we have no control over the design t_1, \dots, t_n and we focus on the convergence of the estimator towards the projection x^\dagger .

Let $\{b_i; \phi_i, \psi_i\}_{i=1, \dots, n}$ be a singular system for the linear operator A_n , that is, $A_n \phi_i = b_i \psi_i$ and $A_n^* \psi_i = b_i \phi_i$ and $b_1^2 \geq \dots \geq b_n^2 > 0$ are the ordered non-zero eigenvalues of the self-adjoint operator $A_n^* A_n$. The ϕ_i 's (resp. ψ_i 's) form an orthonormal system of \mathcal{K}_n^\perp (resp.

\mathbb{R}^n).

In this framework, the available information on x_0 consists in a noisy version of $A_n x_0$. As a result, estimating the part of x_0 lying in \mathcal{K}_n is impossible, based only on the observations. The best approximation of x_0 one can get without prior information is the orthogonal projection of x_0 onto \mathcal{K}_n^\perp . This projection, noted x^\dagger , is called *best approximate solution* and is obtained as the image of $A_n x_0$ through the generalized Moore-Penrose inverse operator $A_n^\dagger = (A_n^* A_n)^\dagger A_n^*$, where $(A_n^* A_n)^\dagger$ denotes the inverse of $A_n^* A_n$, restricted to \mathcal{K}_n^\perp . By construction, the generalized Moore-Penrose inverse A_n^\dagger can also be defined as the operator for which $\{b_i^{-1}; \psi_i, \phi_i\}_{i=1, \dots, n}$ is a singular system. We refer to [9] for further details.

Searching for a solution in the subspace \mathcal{K}_n^\perp allows to reduce the number of regressors to n . Then, estimating x^\dagger can be made using a classical linear regression framework where the number of regressors is equal to the dimension of the observation. Decomposing the observation in the singular basis $\{\psi_i\}_{i=1, \dots, n}$ leads to the following model

$$y_i = b_i x_i + \varepsilon_i, i = 1, \dots, n,$$

where we set $y_i = \langle y, \psi_i \rangle_n$, $\varepsilon_i = \langle \varepsilon, \psi_i \rangle_n$ and $x_i = \langle x_0, \phi_i \rangle$. It now suffices to divide each term by the known singular value b_i to observe the coefficient x_i , up to a noise term $\eta_i := b_i^{-1} \varepsilon_i$. Equivalently, this is obtained by applying the Moore-Penrose inverse A_n^\dagger in the model (1). We thus consider the function $y^\dagger = A_n^\dagger y \in \mathcal{K}_n^\perp$, defined as the inverse image of y through A_n with minimal norm. Identifying y^\dagger with the vector of its coefficients $y_i^\dagger = b_i^{-1} y_i$ in the basis $\{\phi_i\}_{i=1, \dots, n}$, we obtain

$$y_i^\dagger = x_i + \eta_i, i = 1, \dots, n. \quad (2)$$

The covariance matrix of the noise $\eta = (\eta_1, \dots, \eta_n)'$ is diagonal in this model, as we have $\mathbb{E}(\eta_i \eta_j) = n^{-1} b_i^{-1} b_j^{-1} \sigma^2 \langle \psi_i, \psi_j \rangle_n$ which is null for all $i \neq j$ and equal to $\sigma_i^2 := \sigma^2 b_i^{-2} / n$ if $i = j$. Thus, the model can be interpreted as a linear regression model with heteroscedastic noises, the variances σ_i^2 being inversely proportional to the eigenvalues b_i^2 . In the case where ε in the original model (1) is Gaussian with distribution $\mathcal{N}(0, \sigma^2 I)$, the noises η_i remain Gaussian in (2).

This representation points out the effect of the decay of the singular values b_i on the noise level, making the problem ill-posed. To control the noise with a too large variance σ_i^2 , a solution is to consider weighted versions of y^\dagger . For some filter $\lambda = (\lambda_1, \dots, \lambda_n)'$, note $\hat{x}(\lambda) \in \mathcal{K}_n^\perp$ the function defined by $\langle \hat{x}(\lambda), \phi_i \rangle = \lambda_i y_i^\dagger$ for $i = 1, \dots, n$. Filter-based methods aim to cancel out the high frequency noises by allocating low weights to the components y_i^\dagger corresponding to small singular values. A widely used example is the

Tikhonov regularization, with weights of the form $\lambda_i = (1 + \tau\sigma_i^2)^{-1}$ for some $\tau > 0$. The Tikhonov solution can be expressed as the minimizer of the functional

$$\|y - A_n x\|^2 + \tau \|x\|^2, \quad x \in \mathcal{X},$$

which makes the method particularly convenient in cases where the SVD of $A_n^* A_n$ or the coefficients y_i^\dagger are not easily computable. We refer to [3] and [20] for further details.

Another common filter-based method is the *truncated singular value decomposition* or *spectral cut-off* studied in [2], [9] and [11]. An estimator of x_0 is obtained as a truncated version of y^\dagger , where all coefficient y_i^\dagger corresponding to arbitrarily small singular values are replaced by 0. This approach can be viewed as a principal component analysis, where only the highly explanatory directions are selected. The spectral cut-off estimator is associated to filter factors of the form $\lambda_i = \mathbb{1}\{i \leq k\}$, where $\mathbb{1}\{\cdot\}$ denotes the indicator function and k is a bandwidth to be determined. Data-driven methods for selecting suitable values of k are discussed in [3], [4], [11], [21] and [22].

A natural way to generalize the spectral cut-off procedure is to enlarge the class of estimators by considering non-ordered truncated versions of y^\dagger , as made in [14], [15] or [16] (see also Examples 1 and 2 in [5]). This approach reduces to a model selection issue where each model is identified with a set of indices $m \subset \{1, \dots, n\}$. Precisely, for m a given model, define $\hat{x}_m \in \mathcal{K}_n^\perp$ as the orthogonal projection of y^\dagger onto $\mathcal{X}_m := \text{span}\{\phi_i, i \in m\}$, that is, \hat{x}_m satisfies

$$\langle \hat{x}_m, \phi_i \rangle = \begin{cases} y_i^\dagger & \text{if } i \in m, \\ 0 & \text{otherwise.} \end{cases}$$

The objective is to find a model m that makes the expected risk $\mathbb{E}\|\hat{x}_m - x_0\|^2$ small. The computation of the estimator no longer relies on the choice of one parameter $k \in \{1, \dots, n\}$ as for spectral cut-off, but on the choice of a set of indices $m \subset \{1, \dots, n\}$, which increases the number of possibilities. In particular, this approach allows non-monotonic collections of filters that may perform better than decreasing sequences obtained by spectral cut-off. To see this, write the bias-variance decomposition of the estimator \hat{x}_m for a deterministic model m :

$$\mathbb{E}\|\hat{x}_m - x_0\|^2 = \mathbb{E}\|x_0 - x^\dagger\|^2 + \sum_{i \notin m} x_i^2 + \sum_{i \in m} \sigma_i^2.$$

In these settings, it appears that in order to minimize the risk, best is to select indices i for which the component x_i^2 is larger than the noise level σ_i^2 . A proper choice of filter should depend on both the variance σ_i^2 and the coefficient x_i^2 . Consequently, the resulting sequence $\{\lambda_i\}_{i=1, \dots, n}$ has no reason of being a decreasing function of σ_i^2 if some coefficients x_i^2 are large enough to compensate for a large variance.

3 Non-ordered variable selection

3.1 Threshold regularization

The construction of the estimator by non-ordered variable selection reduces to finding a proper set m . Following the discrepancy principle, an optimal value for m (minimizing the risk) is obtained by keeping small simultaneously the bias term $\sum_{i \notin m} x_i^2$ and the variance term $\sum_{i \in m} \sigma_i^2$ in the expression of the risk $\mathbb{E} \|\hat{x}_m - x_0\|^2$. Following the previous argument, a minimizer of the risk $\mathbb{E} \|\hat{x}_m - x_0\|^2$ is obtained by selecting only the indices i for which the coefficient x_i^2 is larger than the noise level σ_i^2 . An optimal model is thus given by $m^* := \{i : x_i^2 \geq \sigma_i^2\}$. The coefficients x_i being unknown to the practitioner, the optimal set m^* can not be computed in practical cases. For this reason it will be referred to as an *oracle*.

We shall now provide a model \hat{m} constructed from the available information, that mimics the oracle m^* . Fixing a threshold on the coefficients x_i being impossible, we propose to use a threshold on the coefficients y_i^\dagger . Precisely, consider the set

$$\hat{m} = \left\{ i : y_i^{\dagger 2} \geq 4\sigma_i^2 \mu_i \right\},$$

for $\{\mu_i\}_{i=1,\dots,n}$ a sequence of positive parameters to be chosen. Obviously, the behavior of the resulting estimator $\hat{x}_{\hat{m}}$ relies on the choice of the sequence $\{\mu_i\}_{i=1,\dots,n}$: the larger the μ_i 's, the more sparse is $\hat{x}_{\hat{m}}$. It must be chosen so that the resulting set \hat{m} contains only the indices i for which the noise level is small compared to the actual value of x_i . Although, the only knowledge of the observations y_i^\dagger and the variances σ_i^2 makes it a difficult task.

There exist general filter-based methods that can be applied to arbitrary classes of filter estimators. One example is the *unbiased risk estimation* discussed in [5], which defines an estimator of x_0 via the minimization of an unbiased estimation of the risk, over an arbitrary set of filters. When restricted to the class of binary filters $\lambda_i \in \{0, 1\}$, unbiased risk estimation reduces to minimizing over \mathcal{M} the criterion

$$m \mapsto \|y^\dagger - \hat{x}_m\|^2 + 2 \sum_{i \in m} \sigma_i^2.$$

The minimum can be shown to be reached for the set $m = \{i : y_i^{\dagger 2} \geq 2\sigma_i^2\}$, which corresponds to taking $\mu_i = 1/2$ in our method. This choice is shown to be asymptotically efficient in Proposition 2 in [5], although additional restrictions are made on the λ_i 's which we intend to relax here in an asymptotic framework. If these conditions are not met, the accuracy of the choice $\mu_i = 1/2$ is not clear. We investigate in the next section a different choice for μ_i which turns out to be nearly optimal in a general framework.

In a general point of view, the estimator $\hat{x}_{\hat{m}}$ can be obtained via a minimization procedure, using a BIC-type criterion for heteroscedastic models,

$$\hat{x}_{\hat{m}} = \operatorname{argmin}_{x \in \mathcal{X}} \left\{ \|y^\dagger - x\|^2 + 4 \sum_{i=1}^n \sigma_i^2 \mu_i \mathbb{1}\{\langle x, \phi_i \rangle \neq 0\} \right\}.$$

In a certain way, this can be seen as a hard-thresholding version of the estimator considered in [16], obtained with a ℓ^1 penalty. However, expressing the estimator as the solution to a minimization equation does not ease the computation. The method requires in any case calculation of the SVD of $A_n^* A_n$ and the coefficients y_i^\dagger , which may be computationally expensive. On the other hand, the computation of the estimator is simple once the decomposition of y^\dagger in the SVD of $A_n^* A_n$ is known, as it suffices to compare each coefficient y_i^\dagger to the threshold $4\sigma_i^2 \mu_i$.

3.2 Oracle inequalities

In the definition of \hat{m} , the choice of the parameters μ_i is crucial. Too large values of μ_i will result in an under-adjustment, keeping too few relevant components y_i^\dagger to estimate x_0 . On the contrary, a small value of μ_i increases the probability of selecting a component y_i^\dagger that is highly affected with noise. Thus, it is essential to find a good balance between these two types of errors. In the next theorem, we provide a nearly optimal choice for the parameters μ_i , under the condition that ε has finite exponential moments.

For $i = 1, \dots, n$, note $\gamma_i := \eta_i^2 / \sigma_i^2 = n\varepsilon_i^2 / \sigma^2$. We make the following assumption.

A1. There exist $K, \beta > 0$ such that $\forall t > 0, \forall i = 1, \dots, n, \mathbb{P}(\gamma_i > t) \leq K e^{-t/\beta}$.

In a Gaussian model, the γ_i 's have χ^2 distribution with one degree of freedom. The condition A1 holds for any $\beta > 2$, taking $K = \sqrt{1 - 2/\beta}$.

Theorem 3.1 *Assume that the condition A1 holds. Set $\mu_i = \max\{\beta \log(n^2 \sigma_i^2), 0\}$, the estimator $\hat{x}_{\hat{m}}$ satisfies*

$$\mathbb{E}\|\hat{x}_{\hat{m}} - x^\dagger\|^2 \leq \mathbb{E}\|\hat{x}_{m^*} - x^\dagger\|^2 + (K_1 \log n + K_2) \sum_{i \in m^*} \sigma_i^2 + \frac{K_3}{n},$$

with $K_1 = 12\beta$, $K_2 = 2 + \beta \log \|x^\dagger\|^2$ and $K_3 = 2K\beta$.

Remark 1. This theorem establishes a non-asymptotic oracle inequality with exact constant. The residual term is similar to that in Corollary 1 in [14]. The fact that the term $\|x^\dagger\|$ depends on n is not problematic here as it can in any case be bounded by the

norm of x_0 .

Remark 2. The method requires knowledge of the operator A_n , the variance σ^2 and the constant β in the condition A1. Note however that knowing the constant K is not necessary to build the estimator.

Remark 3. The set \hat{m} contains all indices i for which $\sigma_i^2 \leq 1/n^2$, as we have in this case $\mu_i = 0$. This suggests that the error caused by wrongfully selecting indices i for which the variance is smaller than $1/n^2$ is negligible, regardless of the value of y_i^\dagger .

Remark 4. In an asymptotic concern, the accuracy of the result stated in Theorem 3.1 relies on the convergence rate of the residual term to zero, compared to the risk of the oracle. The residual term $\sum_{i \in m^*} \sigma_i^2$ is actually the variance term in the bias-variance decomposition of \hat{x}_{m^*} , and therefore, it is bounded by the risk of the oracle. As a result, the estimator $\hat{x}_{\hat{m}}$ is shown to reach at least the same rate of convergence as the oracle, up to a logarithmic term, which warrants good adaptivity properties. The logarithmic term vanishes in the convergence rate if the bias term $\sum_{i \notin m^*} x_i^2$ dominates in the risk of the \hat{x}_{m^*} . Precisely, the oracle inequality is asymptotically exact as soon as the residual term $\log n \sum_{i \in m^*} \sigma_i^2$ is negligible compared to the bias term $\sum_{i \notin m^*} x_i^2$. In this case, it follows from Theorem 3.1 that

$$\mathbb{E} \|\hat{x}_{\hat{m}} - x^\dagger\|^2 = (1 + o(1)) \mathbb{E} \|\hat{x}_{m^*} - x^\dagger\|^2.$$

Of course, this condition is hard to verify in practice and assuming it is true reduces to make strong regularity assumptions on the asymptotic behavior of x_0 and A_n . In a non-asymptotic framework, the theorem warrants that the estimator $\hat{x}_{\hat{m}}$ is close to the oracle as soon as the variance term $\sum_{i \in m^*} \sigma_i^2$ is small compared to the bias term $\sum_{i \notin m^*} x_i^2$ in the bias-variance decomposition of the oracle.

The estimator $\hat{x}_{\hat{m}}$ being built using binary filters $\lambda_i \in \{0, 1\}$, it is natural to measure its efficiency by comparing its risk to that of the best linear estimator in this class. Nevertheless, we see in the next corollary that a similar oracle inequality holds if we consider the oracle in the maximal class of filters, that is, allowing the λ_i 's to take any real value.

Corollary 3.2 *Assume that the condition A1 holds, the estimator $\hat{x}_{\hat{m}}$ of Theorem 3.1 satisfies*

$$\mathbb{E} \|\hat{x}_{\hat{m}} - x^\dagger\|^2 \leq K_4 \log n \inf_{\lambda \in \mathbb{R}^n} \mathbb{E} \|\hat{x}(\lambda) - x^\dagger\|^2 + \frac{K_5}{n},$$

for some constants K_4, K_5 independent of n .

This result is a straightforward consequence of Lemma 5.2 in the Appendix, where it is shown that the oracle in the class of binary filters $\lambda_i \in \{0, 1\}$ achieves the same rate of convergence up to a factor 2, as the best filter estimator obtained with non-random values of λ . The class of unrestricted binary filters leads to a simple solution while it induces a slight loss of efficiency compared to the maximal class.

Interest of oracles lies in the fact that the best estimator in a given class will often reach the optimal rate of convergence. In many situations, comparing the risk of the estimator to that of an oracle might be sufficient to deduce optimality results, as well as adaptivity properties, as discussed in [3]. In the literature of inverse problems, rates of convergence of oracles are obtained under regularity conditions on the map x_0 and the spectrum of A_n . These conditions can be gathered into a single assumption, generally referred to as *source condition*, relating the behavior of x_0 to the regularity of the operator A_n (see for instance [2], [9] or [10]). Another point of view widely adopted in the literature is the *minimax* approach (see [3]), aiming to determine the behavior the worst possible value of x_0 in a given class of functions. Typically, the condition can be a polynomial decay of the coefficients x_i , which reduces to assuming that x_0 lies in the unit ball in a proper Besov space. For rates of convergence with a minimax approach, we refer to [1], [7] and [17]. In our framework, rates of convergence for $\hat{x}_{\hat{m}}$ can be deduced from Theorem 2 in [14], under a polynomial decay of the coefficients x_i and the eigenvalues b_i .

4 Regularization with unknown operator

In many actual situations, the operator A_n is not precisely known. In this section, we consider the framework where the operator A_n is observed independently from y . This situation is treated in [6], [8] or [13]. The method discussed in the previous section does not apply for such problems since it requires complete knowledge of the operator A_n . As in [6], we assume that the eigenvectors ϕ_i and ψ_i are known. This seemingly strong assumption is actually met in many situations, for instance if the problem involves convolution or differential operators which can be decomposed in Fourier basis (see also the examples in [3]). Thus, only the eigenvalues b_i are unknown and we assume they are observed independently of y , with a centered noise ξ_i with known variance $s^2 > 0$:

$$\hat{b}_i = b_i + \xi_i, \quad i = 1, \dots, n.$$

The method discussed in this paper is different according to whether the eigenvalues are known exactly or observed with a noise. Thus, we need to assume here that s is positive and the known operator framework can not be seen as a particular case. Moreover, we assume the ξ_i 's are independent and satisfy the two following conditions.

A2. There exist $K', \beta' > 0$ such that $\forall t > 0, \forall i = 1, \dots, n, \mathbb{P}(\xi_i^2/s^2 > t) \leq K'e^{-t/\beta'}$.

A3. There exist $C, \alpha > 0$ such that $\forall i = 1, \dots, n, \min\{\mathbb{P}(\xi_i < -\alpha s), \mathbb{P}(\xi_i > \alpha s)\} \geq C$.

As discussed previously, the condition A2 means that the ξ_i 's have finite exponential moments. The condition A3 is hardly restrictive, and is fulfilled for instance as soon as the ξ_i 's are identically distributed. As we shall see in the sequel, the method requires knowledge of the constant α (or at least an upper bound for it), but no information on the constants β', K' or C is needed to build the estimator.

Knowing the eigenvectors of $A_n^*A_n$ allows us to write the model in the form

$$y_i = b_i x_i + \varepsilon_i, i = 1, \dots, n.$$

In our framework where the actual eigenvalues b_i are unknown, a natural estimator of each component x_i is obtained by $\tilde{y}_i = \hat{b}_i^{-1} y_i$, provided that $\hat{b}_i \neq 0$. However, it is clear that this estimate is not satisfactory if \hat{b}_i is far from the true value (consider for instance the extreme case where $\hat{b}_i = 0$ or if \hat{b}_i and b_i are of opposite signs). Actually, the naive estimator \hat{b}_i^{-1} can not be used efficiently to estimate b_i^{-1} because it may have an infinite variance. In [6], the authors fix a threshold w the estimate can not exceed and consider an estimator of b_i^{-1} equal to \hat{b}_i^{-1} if $|\hat{b}_i| > 1/w$ and null otherwise. As we will see below, we use the same idea here, although the threshold fixed on the \hat{b}_i 's is implicitly part of the variable selection process.

We can reasonably assume that null values of \hat{b}_i do not provide any relevant information and can not be used to estimate x_0 . Thus, to avoid considering trivial situations, we assume that all \hat{b}_i are non-zero. In all generality, the \tilde{y}_i 's can be viewed as noisy observations of x_i by writing

$$\tilde{y}_i = x_i + \tilde{\eta}_i, i = 1, \dots, n,$$

with $\tilde{y}_i = \hat{b}_i^{-1} \langle y, \psi_i \rangle_n$ and $\tilde{\eta}_i = \hat{b}_i^{-1}(\varepsilon_i - \xi_i x_i)$, where we recall $\varepsilon_i = \langle \varepsilon, \psi_i \rangle_n$. As in the previous section, we propose a threshold procedure to filter out the observations \tilde{y}_i that are potentially highly contaminated with noise. Here, the noise $\tilde{\eta}_i$ is more difficult to deal with because it depends on the unknown coefficient x_i .

Our objective is to find an optimal variable selection criterion conditionally to the \hat{b}_i 's. In order to do so, we consider a framework where the \hat{b}_i 's are observed once and for all, and are treated as non-random. Thus, we define as an oracle, a model m_ξ^* minimizing the conditional risk $\mathbb{E}_\xi \|\hat{x}_m - x^\dagger\|^2$, where $\mathbb{E}_\xi(\cdot)$ denotes the expectation knowing $\xi = (\xi_1, \dots, \xi_n)'$. Following a similar argument as in the previous section, a model minimizing the conditional risk contains only the indices i for which the coefficient x_i^2 is larger than the noise level. Hence, we may define $m_\xi^* = \{i : x_i^2 > \mathbb{E}_\xi(\tilde{\eta}_i^2)\}$. A notable difference here is that the noise $\tilde{\eta}_i$ actually depends on the value x_i . Let $\hat{\sigma}_i^2 = n^{-1} \hat{b}_i^{-2} \sigma^2$, we can calculate

the conditional expectation of $\tilde{\eta}_i^2$, given by $\mathbb{E}_\xi(\tilde{\eta}_i^2) = \hat{\sigma}_i^2 + \hat{b}_i^{-2}\xi_i^2x_i^2$. After simplifications, it appears that the optimal model conditionally to the ξ_i 's can be expressed in the two following explicit forms

$$m_\xi^* = \left\{ i : 2|\hat{b}_i| > \frac{\sigma^2}{n|b_i|x_i^2} + |b_i| \right\} = \left\{ i : x_i^2 > \frac{\sigma^2}{n(\hat{b}_i^2 - \xi_i^2)}, |\hat{b}_i| > \frac{|b_i|}{2} \right\}.$$

In the first expression, we see that the oracle selects indices i for which the observation \hat{b}_i exceeds a certain value depending on both x_i and b_i . Interestingly, components \tilde{y}_i corresponding to observations \hat{b}_i smaller than half the true eigenvalue b_i are not selected in the oracle, regardless of the coefficient x_i . Here again, the optimal model m_ξ^* can not be used in practical cases since it involves the unknown values x_i and ξ_i . We can only try to mimic the optimal threshold, based on the observations \tilde{y}_i and \hat{b}_i . Consider the set

$$\hat{m}_\xi = \left\{ i : \tilde{y}_i^2 > 8\hat{\sigma}_i^2\nu_i, |\hat{b}_i| > \alpha s \right\},$$

where $\{\nu_i\}_{i=1,\dots,n}$ are parameters to be chosen and α is the constant defined in A3. With this definition, only the indices for which the observation \hat{b}_i is larger than a certain value, namely αs , are selected. This conveys the idea discussed in [6], that when b_i is small compared to the noise level, the observation \hat{b}_i is potentially mainly noise. Remark however that in [6], the lower limit for the observed eigenvalues is $s \log^2(1/s)$, while in our method, it is chosen of the same order as the standard deviation s .

Define the set $M = \{i : |b_i| < 2\alpha s\}$.

Theorem 4.1 *Assume that the condition A1 holds. The threshold estimator obtained with $\nu_i = \max\{\beta \log(n^2\hat{\sigma}_i^2), 0\}$ satisfies,*

$$\mathbb{E}_\xi \|\hat{x}_{\hat{m}_\xi} - x^\dagger\|^2 \leq (K'_1 \log n + K'_2) \mathbb{E}_\xi \|\hat{x}_{m_\xi^*} - x^\dagger\|^2 + \sum_{i \in M} x_i^2 + \kappa(\xi),$$

with $K'_1 = \max\{18\beta, 4\alpha^{-2}\beta'\}$, $K'_2 = \max\{9(\beta \log \|x^\dagger\|^2 + 1), 1\}$, and

$$\kappa(\xi) = \frac{4K\beta}{n} + 4 \sum_{i \notin m_\xi^*} \frac{\xi_i^2 x_i^2}{\alpha^2 s^2} \mathbb{1}\{\xi_i^2 > s^2 \beta' \log n\}.$$

Moreover, if A2 holds, $\mathbb{E}(\kappa(\xi)) = O(n^{-1} \log n)$.

The main interest of this result lies in the fact that it provides an oracle inequality, conditionally to the \hat{b}_i 's. In particular, the conditional oracle $\hat{x}_{m_\xi^*}$ is more efficient than the estimator obtained by minimizing the expected risk $m \mapsto \mathbb{E} \|\hat{x}_m - x^\dagger\|^2$, since the

optimal set m_ξ^* is allowed to depend on the ξ_i 's. We see that the estimator $\hat{x}_{\hat{m}_\xi}$ performs almost as well as the conditional oracle. Indeed, the residual term $\kappa(\xi)$ is independent from ξ with high probability, and its expectation is negligible under A2 as pointed out in the theorem. The non-random term $\sum_{i \in M} x_i^2$ is small if the eigenvalues b_i are observed with a good precision, i.e. if the variance s^2 is small. Moreover, this term can be shown to be of the same order as the risk under the condition A3.

Corollary 4.2 *If the conditions A1, A2 and A3 hold, the threshold estimator defined in Theorem 4.1 satisfies*

$$\mathbb{E} \|\hat{x}_{\hat{m}_\xi} - x^\dagger\|^2 \leq K'_4 \log n \mathbb{E} \|\hat{x}_{m_\xi^*} - x^\dagger\|^2 + \frac{K'_5 \log n}{n},$$

for some constants K'_4 and K'_5 independent from n and s^2 .

With a noisy operator, we manage to provide an estimator that achieves the rate of convergence of the conditional oracle, regardless of the precision of the approximation of the spectrum of A_n . Indeed, the constants K'_4 and K'_5 in Corollary 4.2 do not involve the variance s^2 of ξ . Actually, the variance only plays a role in the accuracy of the oracle. The result is non-asymptotic and requires no assumption on s^2 .

5 Appendix

5.1 Technical lemmas

Lemma 5.1 *Assume the condition A1 holds. We have*

- $\mathbb{E}((\eta_i^2 - x_i^2) \mathbb{1}\{i \in \hat{m}\}) \leq 2K\beta\sigma_i^2 e^{-\mu_i/\beta}$.
- $\mathbb{E}((x_i^2 - \eta_i^2) \mathbb{1}\{i \notin \hat{m}\}) \leq \sigma_i^2(6\mu_i + 2)$.

Proof. Using the inequality $(a + b)^2 \leq 2a^2 + 2b^2$, we find that $\eta_i^2 - x_i^2 \leq 2\eta_i^2 - y_i^{\dagger 2}/2$. By definition of \hat{m} , we get

$$(\eta_i^2 - x_i^2) \mathbb{1}\{i \in \hat{m}\} \leq 2\sigma_i^2(\gamma_i - \mu_i) \mathbb{1}\{i \in \hat{m}\} \leq 2\sigma_i^2(\gamma_i - \mu_i) \mathbb{1}\{\gamma_i \geq \mu_i\},$$

where we used that $X \leq X \mathbb{1}\{X \geq 0\}$. We finally obtain for all $i \notin m^*$,

$$\mathbb{E}((\eta_i^2 - x_i^2) \mathbb{1}\{i \in \hat{m}\}) \leq 2\sigma_i^2 \int_0^\infty \mathbb{P}(\gamma_i \geq t + \mu_i) dt \leq 2K\beta\sigma_i^2 e^{-\mu_i/\beta},$$

as a consequence of A1. For the second part of the lemma, write $x_i^2 - \eta_i^2 = y_i^{\dagger 2} - 2\eta_i y_i^\dagger$ which is bounded by $3y_i^{\dagger 2}/2 + 2\eta_i^2$, using the inequality $2ab \leq 2a^2 + b^2/2$. This leads to

$$\mathbb{E}((x_i^2 - \eta_i^2) \mathbb{1}\{i \notin \hat{m}\}) \leq \sigma_i^2(6\mu_i + 2).$$

Lemma 5.2

$$\inf_{m \in \mathcal{M}} \mathbb{E} \|\hat{x}_m - x^\dagger\|^2 \leq 2 \inf_{\lambda \in \mathbb{R}^n} \mathbb{E} \|\hat{x}(\lambda) - x^\dagger\|^2.$$

Proof. The minimal values of the expected risks can be calculated explicitly in the two classes considered here. Minimizing over \mathbb{R}^n the function $\lambda \mapsto \mathbb{E} \|\hat{x}(\lambda) - x^\dagger\|^2$, we find that the optimal value of λ_i is reached for $\lambda_i^* = x_i^2 / (x_i^2 + \sigma_i^2)$. On the other hand, we know that $m \mapsto \mathbb{E} \|\hat{x}_m - x^\dagger\|^2$ reaches its minimum at $m^* = \{i : x_i^2 \geq \sigma_i^2\}$, yielding

$$\inf_{\lambda \in \mathbb{R}^n} \mathbb{E} \|\hat{x}(\lambda) - x^\dagger\|^2 = \sum_{i=1}^n \frac{x_i^2 \sigma_i^2}{x_i^2 + \sigma_i^2} \quad \text{and} \quad \inf_{m \in \mathcal{M}} \mathbb{E} \|\hat{x}_m - x^\dagger\|^2 = \sum_{i \in m^*} \sigma_i^2 + \sum_{i \in m^*} x_i^2.$$

By definition, if $i \in m^*$, $2x_i^2 / (x_i^2 + \sigma_i^2) \geq 1$. In the same way, $2\sigma_i^2 / (x_i^2 + \sigma_i^2) \geq 1$, for all $i \notin m^*$. We conclude by summing all the terms.

Lemma 5.3 *Assume the condition A1 holds. We have, for all $i = 1, \dots, n$,*

- $\mathbb{E}_\xi ((\tilde{\eta}_i^2 - x_i^2) \mathbf{1}\{i \in \hat{m}_\xi\}) \leq 4K\beta \hat{\sigma}_i^2 e^{-\nu_i/\beta} + \frac{4\xi_i^2 x_i^2}{\alpha^2 s^2}.$
- $\mathbb{E}_\xi ((x_i^2 - \tilde{\eta}_i^2) \mathbf{1}\{i \notin \hat{m}_\xi\}) \leq 9\hat{\sigma}_i^2 \nu_i + 8\mathbb{E}_\xi(\tilde{\eta}_i^2) + x_i^2 \mathbf{1}\{|\hat{b}_i| \leq \alpha s\}.$

Proof. Remark that $\tilde{\eta}_i^2 = \hat{b}_i^{-2} (\varepsilon_i - \xi_i x_i)^2 \leq 2\hat{b}_i^{-2} \varepsilon_i^2 + 2\hat{b}_i^{-2} \xi_i^2 x_i^2$. Using that $x_i^2 \geq \tilde{y}_i^2 / 2 - \tilde{\eta}_i^2$, we deduce

$$\tilde{\eta}_i^2 - x_i^2 \leq 4\hat{b}_i^{-2} \varepsilon_i^2 + 4\hat{b}_i^{-2} \xi_i^2 x_i^2 - \frac{\tilde{y}_i^2}{2}.$$

Writing $\hat{m}_\xi = \{\tilde{y}_i^2 > 8\hat{\sigma}_i^2 \nu_i\} \cap \{|\hat{b}_i| > \alpha s\}$, we find

$$(\tilde{\eta}_i^2 - x_i^2) \mathbf{1}\{i \in \hat{m}_\xi\} \leq 4\hat{\sigma}_i^2 (\gamma_i - \nu_i) \mathbf{1}\{\gamma_i \geq \nu_i\} + 4\hat{b}_i^{-2} \xi_i^2 x_i^2 \mathbf{1}\{|\hat{b}_i| > \alpha s\},$$

where we recall that $\gamma_i = n\varepsilon_i^2 / \sigma^2$. Clearly, $\hat{b}_i^{-2} \mathbf{1}\{|\hat{b}_i| > \alpha s\} < \alpha^{-2} s^{-2}$ and the result follows using the condition A1. For the second part of the lemma, remark that the complement of \hat{m}_ξ is $\{\tilde{y}_i^2 \leq 8\hat{\sigma}_i^2 \nu_i, |\hat{b}_i| > \alpha s\} \cup \{|\hat{b}_i| \leq \alpha s\}$. Using the inequality $x_i^2 - \tilde{\eta}_i^2 \leq (1 + \theta^{-1})\tilde{y}_i^2 + \theta\tilde{\eta}_i^2$ for $\theta = 8$, we get

$$(x_i^2 - \tilde{\eta}_i^2) \mathbf{1}\{i \notin \hat{m}_\xi\} \leq 9\hat{\sigma}_i^2 \nu_i + 8\tilde{\eta}_i^2 + x_i^2 \mathbf{1}\{|\hat{b}_i| \leq \alpha s\}.$$

Lemma 5.4 *If A2 holds, we have*

$$\xi_i^2 \leq s^2 \beta' \log n + \xi_i^2 \mathbf{1}\{\xi_i^2 > s^2 \beta' \log n\},$$

with $\mathbb{E}(\xi_i^2 \mathbf{1}\{\xi_i^2 > s^2 \beta' \log n\}) = O(n^{-1} \log n)$.

Proof. Write $\xi_i^2 \leq s^2 \beta' \log n \mathbf{1}\{\xi_i^2 \leq s^2 \beta' \log n\} + \xi_i^2 \mathbf{1}\{\xi_i^2 > s^2 \beta' \log n\}$. To bound the first term, we use the crude inequality $\mathbf{1}\{\xi_i^2 \leq s^2 \beta' \log n\} \leq 1$. For the second term, we have as a consequence of A2,

$$\begin{aligned} \mathbb{E}(\xi_i^2 \mathbf{1}\{\xi_i^2 > s^2 \beta' \log n\}) &= \int_0^\infty \mathbb{P}(\xi_i^2 \mathbf{1}\{\xi_i^2/s^2 > \beta' \log n\} > t) dt \\ &= s^2 \beta' \log n \mathbb{P}(\xi_i^2/s^2 > \beta' \log n) + s^2 \int_{\beta' \log n}^\infty \mathbb{P}(\xi_i^2/s^2 > t) dt \\ &\leq \frac{K' \beta' s^2 (1 + \log n)}{n}. \end{aligned}$$

5.2 Proofs

Proof of Theorem 3.1. Write

$$\|\hat{x}_{\hat{m}} - x_0\|^2 = \|\hat{x}_{m^*} - x_0\|^2 + \sum_{i \notin m^*} (\eta_i^2 - x_i^2) \mathbf{1}\{i \in \hat{m}\} + \sum_{i \in m^*} (x_i^2 - \eta_i^2) \mathbf{1}\{i \notin \hat{m}\}.$$

The objective is to bound the terms $\mathbb{E}((\eta_i^2 - x_i^2) \mathbf{1}\{i \in \hat{m}\})$ and $\mathbb{E}((x_i^2 - \eta_i^2) \mathbf{1}\{i \notin \hat{m}\})$. First, assume that $\sigma_i^2 > 1/n^2$, i.e. $\mu_i = \beta \log(n^2 \sigma_i^2)$. By Lemma 5.1, we know that

$$\mathbb{E}((\eta_i^2 - x_i^2) \mathbf{1}\{i \in \hat{m}\}) \leq 2K\beta\sigma_i^2 e^{-\mu_i/\beta} \leq \frac{2K\beta}{n^2}.$$

The same bound holds if $\sigma_i^2 \leq 1/n^2$ with $\mu_i = 0$, as a straight-forward consequence of Lemma 5.1. On the other hand, note that if $i \notin \hat{m}$, then $\mu_i = \beta \log(n^2 \sigma_i^2)$. Lemma 5.1 warrants

$$\mathbb{E}((x_i^2 - \eta_i^2) \mathbf{1}\{i \notin \hat{m}\}) \leq \sigma_i^2 (6\beta \log(n^2 \sigma_i^2) + 2).$$

Since $i \in m^*$, $\log(n^2 \sigma_i^2) \leq 2 \log n + \log \|x^\dagger\|^2$. We conclude by summing all the terms.

Proof of Theorem 4.1. The proof starts as in Theorem 3.1. We have

$$\|\hat{x}_{\hat{m}_\xi} - x^\dagger\|^2 = \|\hat{x}_{m_\xi^*} - x^\dagger\|^2 + \sum_{i \notin m_\xi^*} (\tilde{\eta}_i^2 - x_i^2) \mathbf{1}\{i \in \hat{m}_\xi\} + \sum_{i \in m_\xi^*} (x_i^2 - \tilde{\eta}_i^2) \mathbf{1}\{i \notin \hat{m}_\xi\},$$

and the objective is to bound the conditional expectation of each term separately. Using successively Lemma 5.3 and Lemma 5.4, we get

$$\mathbb{E}_\xi((\tilde{\eta}_i^2 - x_i^2) \mathbf{1}\{i \in \hat{m}_\xi\}) \leq \frac{4K\beta}{n^2} + 4\alpha^{-2} s^{-2} \xi_i^2 x_i^2 \leq \frac{4\beta' \log n}{\alpha^2} x_i^2 + \kappa_i(\xi),$$

with

$$\kappa_i(\xi) = \frac{4K\beta}{n^2} + \frac{4\xi_i^2 x_i^2}{\alpha^2 s^2} \mathbf{1}\{\xi_i^2 > s^2 \beta' \log n\}.$$

By Lemma 5.4, we know that $\kappa(\xi) = \sum_{i \notin m_\xi^*} \kappa_i(\xi)$ is such that

$$\mathbb{E}(\kappa(\xi)) \leq \frac{4(K\beta + 2\alpha^{-2}K'\beta'\|x^\dagger\|^2 \log n)}{n} = O\left(\frac{\log n}{n}\right).$$

On the other hand, Lemma 5.3 gives, for $\theta = 8$,

$$\mathbb{E}_\xi((x_i^2 - \tilde{\eta}_i^2)\mathbf{1}\{i \notin \hat{m}_\xi\}) \leq 9\hat{\sigma}_i^2\nu_i + 8\mathbb{E}_\xi(\tilde{\eta}_i^2) + x_i^2\mathbf{1}\{|\hat{b}_i| \leq \alpha s\}.$$

For all $i \in m_\xi^*$, we know that $|\hat{b}_i| \geq |b_i|/2$. Thus, if $i \in m_\xi^*$, $\mathbf{1}\{|\hat{b}_i| \leq \alpha s\} \leq \mathbf{1}\{i \in M\}$, where we recall $M = \{i : |b_i| < 2\alpha s\}$. We know also that, if $i \in m_\xi^*$, then $\hat{\sigma}_i^2 \leq x_i^2$. Thus, $\nu_i = \beta \log(n^2\hat{\sigma}_i^2) \leq 2\beta \log n + \beta \log\|x^\dagger\|^2$. Noticing that $\hat{\sigma}_i^2 \leq \mathbb{E}_\xi(\tilde{\eta}_i^2)$, we find

$$\mathbb{E}_\xi((x_i^2 - \tilde{\eta}_i^2)\mathbf{1}\{i \notin \hat{m}_\xi\}) \leq (18\beta \log n + 9\beta \log\|x^\dagger\|^2 + 8)\mathbb{E}_\xi(\tilde{\eta}_i^2) + x_i^2\mathbf{1}\{i \in M\}.$$

The result follows by summing all the term, using that the risk of the oracle $\hat{x}_{\hat{m}_\xi}$ is

$$\mathbb{E}_\xi\|\hat{x}_{m_\xi^*} - x^\dagger\|^2 = \sum_{i \notin m_\xi^*} x_i^2 + \sum_{i \in m_\xi^*} \mathbb{E}_\xi(\tilde{\eta}_i^2).$$

Proof of Corollary 4.2. It suffices to show that the term $\sum_{i \in M} x_i^2$ is of the same order as the risk of the oracle. Write

$$\mathbb{E}\|\hat{x}_{m_\xi^*} - x^\dagger\|^2 \geq \sum_{i=1}^n x_i^2 \mathbb{P}(i \notin m_\xi^*) \geq \sum_{i=1}^n x_i^2 \mathbb{P}(|\hat{b}_i| \leq |b_i|/2).$$

For all $i \in M$, the probability $\mathbb{P}(|\hat{b}_i| \leq |b_i|/2)$ is greater than C as a consequence of A3. We deduce $\sum_{i \in M} x_i^2 \leq C^{-1}\mathbb{E}\|\hat{x}_{m_\xi^*} - x^\dagger\|^2$.

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