

Empirical risk minimization as parameter choice rule for general linear regularization methods

Housen Li^a and Frank Werner^{a,b}

^aUniversity of Goettingen, Goettingen, Germany. E-mail: housen.li@mathematik.uni-goettingen.de

^bMax Planck Institute for Biophysical Chemistry, Goettingen, Germany. E-mail: frank.werner@mpibpc.mpg.de

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Abstract. We consider the statistical inverse problem to recover f from noisy measurements $Y = Tf + \sigma\xi$ where ξ is Gaussian white noise and T a compact operator between Hilbert spaces. Considering general reconstruction methods of the form $\hat{f}_\alpha = q_\alpha(T^*T)T^*Y$ with an ordered filter q_α , we investigate the choice of the regularization parameter α by minimizing an unbiased estimate of the predictive risk $\mathbb{E}[\|Tf - T\hat{f}_\alpha\|^2]$. The corresponding parameter α_{pred} and its usage are well-known in the literature, but oracle inequalities and optimality results in this general setting are unknown. We prove a (generalized) oracle inequality, which relates the direct risk $\mathbb{E}[\|f - \hat{f}_{\alpha_{\text{pred}}}\|^2]$ with the oracle prediction risk $\inf_{\alpha>0} \mathbb{E}[\|Tf - T\hat{f}_\alpha\|^2]$. From this oracle inequality we are then able to conclude that the investigated parameter choice rule is of optimal order in the minimax sense.

Finally we also present numerical simulations, which support the order optimality of the method and the quality of the parameter choice in finite sample situations.

Résumé. Nous considérons le problème inverse stochastique de reconstruire f à partir de données bruitées $Y = Tf + \sigma\xi$ où ξ est un bruit blanc et T un opérateur compact entre espaces de Hilbert. Considérant des méthodes de reconstruction générales de la forme $\hat{f}_\alpha = q_\alpha(T^*T)T^*Y$ avec un filtre ordonné q_α , nous examinons le choix du paramètre de régularisation α en minimisant un estimateur non biaisé du risque prédictif $\mathbb{E}[\|Tf - T\hat{f}_\alpha\|^2]$. Le paramètre correspondant α_{pred} et son utilisation sont bien connus dans la littérature mais les inégalités oracles et les résultats d'optimalité dans ce cadre général sont inconnus. Nous prouvons une inégalité oracle (généralisée), qui relie le risque direct $\mathbb{E}[\|f - \hat{f}_{\alpha_{\text{pred}}}\|^2]$ au risque de l'oracle de prédiction $\inf_{\alpha>0} \mathbb{E}[\|Tf - T\hat{f}_\alpha\|^2]$. À partir de cette inégalité oracle nous sommes alors capable de conclure que la règle de choix du paramètre examiné est d'ordre optimale au sens minimax.

Finalement nous présentons aussi des simulations numériques qui confirment l'optimalité de l'ordre de la méthode et la qualité du choix du paramètre dans des situations discrètes.

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1. Introduction

Suppose we want to recover an unknown function $f \in \mathcal{X}$ from noisy measurements

$$Y = Tf + \sigma\xi, \tag{1}$$

where $T : \mathcal{X} \rightarrow \mathcal{Y}$ is an operator between Hilbert spaces \mathcal{X} and \mathcal{Y} , ξ is a standard Gaussian white noise process and $\sigma > 0$ denotes the noise level. In fact, model (1) has to be understood in a weak sense as $\xi \notin \mathcal{Y}$, i.e. for each $y \in \mathcal{Y}$ we have access to observations of the form

$$Y_y := \langle Tf, y \rangle_{\mathcal{Y}} + \sigma \langle \xi, y \rangle_{\mathcal{Y}^* \times \mathcal{Y}},$$

where $\langle \xi, y \rangle_{\mathcal{Y}^* \times \mathcal{Y}} \sim \mathcal{N}(0, \|y\|_{\mathcal{Y}}^2)$ and $\mathbb{E}[\langle \xi, y_1 \rangle_{\mathcal{Y}^* \times \mathcal{Y}} \langle \xi, y_2 \rangle_{\mathcal{Y}^* \times \mathcal{Y}}] = \langle y_1, y_2 \rangle_{\mathcal{Y}}$ for all $y_1, y_2 \in \mathcal{Y}$. Models of the form (1) underly a plentitude of applications, see e.g. O'Sullivan [51], and have been considered by Mathé and Pereverzev [46], Bissantz et al. [8], Ingster et al. [31,32] and Werner [61].

Throughout the paper we will assume that the operator T is injective, compact and Hilbert–Schmidt, i.e. the squares of its singular values are summable. Especially, this implies that its singular values tend to 0 and hence the inversion of T is unstable, i.e. the problem to recover f from (1) is ill-posed and regularization is needed, see Cavalier [11], Engl et al. [22] and the references therein. In the literature many different approaches for the estimation of f can be found, including methods based on a singular value decomposition (SVD) of T (see e.g. [13,33,34,42]), wavelet-vaguelette [21] and vaguelette-wavelet methods [1], and Galerkin-type methods [16].

In this paper we follow a common paradigm and consider regularization methods written in terms of an *ordered filter* $q_\alpha : [0, \|T^*T\|] \rightarrow \mathbb{R}$ parametrized by $\alpha > 0$ (see e.g. Definition 1 for the precise requirements on q_α), meaning that the regularized solution is given by

$$\hat{f}_\alpha := q_\alpha(T^*T)T^*Y. \quad (2)$$

Regularization methods of the form (2) include famous examples like spectral cut-off and Tikhonov regularization, and have been studied extensively in the literature, see Engl et al. [22] and the references therein, and Bissantz et al. [8].

Choosing an appropriate parameter α in (2) is an important problem in regularization theory as it dramatically influences the performance of the estimator \hat{f}_α . Bissantz et al. [8] show that estimators of the form (2) are order-optimal over certain smoothness classes $\mathcal{W} \subset \mathcal{X}$, if the parameter $\alpha = \alpha_*$ is chosen in a reasonable a-priori way (depending on properties of \mathcal{W}). This means that \hat{f}_{α_*} achieves the best possible rate of convergence w.r.t. the *direct risk* $R(\alpha, f) := \mathbb{E}[\|\hat{f}_\alpha - f\|_{\mathcal{X}}^2]$ in these classes. In practice, the parameter α has to be chosen without any knowledge of f (and hence of \mathcal{W}), which makes a-priori parameter choice rules useless. Therefore, *a-posteriori* parameter choice rules are of interest, as they make only use of the data Y and the noise level $\sigma > 0$. As a-posteriori parameter choice rules have to adapt to the unknown properties of \mathcal{W} (and hence of f), this issue is also known as *adaptivity*. For simplicity, we will assume here that σ is known. In practice, the parameter σ can typically be estimated sufficiently fast from the data or the measurement setting (see e.g. [19,29,53]). We will discuss this situation in more detail in Section 6.

A variety of a-posteriori parameter choice rules have been proposed in the literature, including the discrepancy principle [9,17,41,49], generalized cross-validation [24,40,59], the Lepskiĭ-type balancing principle [36,44,48,63] and many more. We refer to Bauer and Lukas [4] for a recent overview and numerical comparison. General adaptivity in statistical inverse problems has also been treated in Goldenshluger [23], Tsybakov [56] and Cavalier et al. [14].

In this paper we deal with a specific method based on empirical risk minimization originally introduced by Mallows [43] for model selection in linear regression and therefore known as *Mallows's C_L* . Consider the *prediction risk* $r(\alpha, f) := \mathbb{E}[\|T(\hat{f}_\alpha - f)\|_{\mathcal{Y}}^2]$. Following Stein [55], we find that an (up to a constant independent of α) unbiased estimator for this quantity is given by

$$\hat{r}(\alpha, Y) := \|T\hat{f}_\alpha\|_{\mathcal{Y}}^2 - 2\langle Y, T\hat{f}_\alpha \rangle_{\mathcal{Y}^* \times \mathcal{Y}} + 2\sigma^2 \text{Trace}(T^*Tq_\alpha(T^*T)). \quad (3)$$

Now the idea is to choose α as a minimizer of $\hat{r}(\alpha, Y)$, i.e.

$$\alpha_{\text{pred}} \in \underset{\alpha > 0}{\text{argmin}} \hat{r}(\alpha, Y).$$

Note that the functional (3) penalizes the misfit between the model \hat{f}_α and the data Y , and furthermore $2\sigma^2 \times \text{Trace}(T^*Tq_\alpha(T^*T))$ penalizes the number of degrees of freedom of the model. We refer to Birgé and Massart [6,7] for details and a discussion of other possible penalty terms in (3).

It is known that choosing $\alpha = \alpha_{\text{pred}}$ in combination with certain regularization schemes leads to an order optimal method w.r.t. the prediction risk $r(\alpha, f)$, see e.g. Li [37], Vogel [57] and Lukas [40]. A very precise result about its performance, which is also a central ingredient of this paper, can be found in the seminal paper by Kneip [35], who proves exponential deviation bounds for $r(\alpha_{\text{pred}}, f)$.

Due to ill-posedness, optimality w.r.t. the prediction risk is however a very weak statement, and consequently we are interested in order optimality w.r.t. the direct risk. This question has hardly been touched in the literature, and to the authors' best knowledge the only result is due to Chernousova and Golubev [15] who restrict to finite dimensional spaces and spectral cut-off regularization. Nevertheless, the choice $\alpha = \alpha_{\text{pred}}$ has successfully been applied in image denoising applications (see e.g. [10,18,39,60]). Moreover, the distributional behavior of α_{pred} has recently been studied by Lucka et al. [38]. There it has been argued that the choice α_{pred} and choices based on unbiased risk minimization in general do not seem suitable for inverse problems. Besides, it remains one of the most popular parameter selection rules, due to its favorable practical performance (cf. [4,15]). In this spirit, we will prove an *oracle inequality* of the form

$$R(\bar{\alpha}, f) \leq \Theta \left(\min_{\alpha > 0} r(\alpha, f) \right) \quad (4)$$

for all $f \in \mathcal{W}$ as $\sigma \searrow 0$ where Θ is some (explicit) functional and $\mathcal{W} \subset \mathcal{X}$ some smoothness class. More specifically, the functional Θ will be such that we can derive order optimality of $\hat{f}_{\alpha_{\text{pred}}}$ under weak assumptions over many classes $\mathcal{W} \subset \mathcal{X}$. Moreover, we provide a general strategy to prove estimates of the form (4) which is of independent interest and might be used for the analysis of other a-posteriori parameter choice rules as well. This makes our analytical methodology substantially different from that in Chernousova and Golubev [15], since the crucial techniques (such as optional stopping of martingales) there do not apply to general regularization schemes. For more details on oracle inequalities in statistical inverse problems we refer to Cavalier et al. [12] and Blanchard et al. [9].

The rest of this paper is organized as follows. In the next section we introduce ordered filter based regularization methods and the empirical parameter choice rule via unbiased prediction risk minimization. The convergence analysis of such a rule is established by means of an oracle inequality in Section 3 with corresponding conclusions on order optimality. In Section 4 we present a general methodology for proving oracle inequalities of the form (4) and apply this methodology for proving the results from Section 3. The performance, as well as the convergence behavior, of the analyzed parameter choice rule is examined by comparison with other empirical parameter choice rules in a simulation study in Section 5. We end this paper with some conclusions in Section 6. Some technical details are deferred to Appendices A and B.

2. Filter based regularization and empirical risk minimization

2.1. Ordered filter based regularization methods

Suppose that \mathcal{X} and \mathcal{Y} are Hilbert spaces, $T : \mathcal{X} \rightarrow \mathcal{Y}$ is an injective and compact Hilbert–Schmidt operator, and ξ in (1) is a standard Gaussian white noise process as described in the Introduction. To simplify the notation we will always assume that $\dim(\mathcal{X}) = \infty$, but stress that the case of finite dimensional \mathcal{X} (and \mathcal{Y}) can be treated similarly. By assumption, there exists a singular value decomposition (SVD) $\{(\sqrt{\lambda_k}, e_k, g_k)\}_{k \in \mathbb{N}}$ of T where $\lambda_1 \geq \lambda_2 \geq \dots > 0$ are the eigenvalues of T^*T , e_1, e_2, \dots are the corresponding normalized eigenvectors, and $g_k = \lambda_k^{-1/2} T e_k$ for $k = 1, 2, \dots$. By introducing the notation $Y_k := \langle g_k, Y \rangle$, $\xi_k := \langle g_k, \xi \rangle$ and $f_k = \langle f, e_k \rangle$, we equivalently transform the model (1) to the Gaussian sequence model

$$Y_k = \sqrt{\lambda_k} f_k + \sigma \xi_k, \quad k = 1, 2, \dots, \text{ with } \xi_k \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1). \quad (5)$$

As mentioned in the Introduction, we focus on regularization methods of the form (2), which by means of (5) can be equivalently formulated as

$$(\hat{f}_\alpha)_k = \sqrt{\lambda_k} q_\alpha(\lambda_k) Y_k, \quad k \in \mathbb{N}. \quad (6)$$

Remark 1. Note that T being Hilbert–Schmidt implies that $\sum_{k=1}^{\infty} \lambda_k < \infty$, and hence T^*Y can be interpreted as a random variable with values in \mathcal{X} as

$$\mathbb{E}[\|T^*\xi\|_{\mathcal{X}}^2] = \mathbb{E}\left[\sum_{k=1}^{\infty} \langle \xi, T e_k \rangle_{\mathcal{Y}}^2\right] = \sum_{k=1}^{\infty} \lambda_k \mathbb{E}[\langle \xi, g_k \rangle_{\mathcal{Y}}^2] < \infty.$$

Consequently, \hat{f}_α as in (2) is well-defined.

Estimators of the form (2) or (6) can be understood as stable approximations of the well-known least squares estimate $\hat{f} := (T^*T)^{-1} T^*Y$ (or $\hat{f}_k = Y_k / \sqrt{\lambda_k}$) in the sense of replacing $(\cdot)^{-1}$ with a function $q_\alpha(\cdot)$. To obtain a well-defined and reasonable regularization method, the functions $q_\alpha(\cdot)$ should satisfy proper conditions. We are particularly interested in case that $q_\alpha(\cdot)$ is an ordered filter.

Definition 1. Let $q_\alpha : [0, \lambda_1] \rightarrow \mathbb{R}$, indexed by $\alpha \in \mathcal{A} \subset \mathbb{R}_+$, be a sequence of functions. We always assume that \mathcal{A} is bounded and closed, equipped with the subspace topology inherited from \mathbb{R}_+ , and that $0 \in \mathcal{A}$.

- (i) The family q_α , $\alpha \in \mathcal{A}$, is called a *filter*, if there exist constants $C'_q, C''_q > 0$ such that for every $\alpha \in \mathcal{A}$ and every $\lambda \in [0, \lambda_1]$

$$\alpha |q_\alpha(\lambda)| \leq C'_q \quad \text{and} \quad \lambda |q_\alpha(\lambda)| \leq C''_q.$$

Table 1
Examples of ordered filters

Method	$q_\alpha(\lambda)$	C'_q	C''_q	v_0	C_v	SVD required
Spectral cut-off	$\frac{1}{\lambda} \mathbf{1}_{[\alpha, \infty)}(\lambda)$	1	1	∞	1	Yes
Tikhonov	$\frac{1}{\lambda + \alpha}$	1	1	1	$v^v(1-v)^{1-v}$	No
m -iterated Tikhonov	$\frac{(\lambda + \alpha)^m - \alpha^m}{\lambda(\lambda + \alpha)^m}$	m	1	m	$(v/m)^v(1-v/m)^{m-v}$	No
Landweber ($\ T\ \leq 1$)	$\sum_{j=0}^{\lfloor 1/\alpha \rfloor - 1} (1 - \lambda)^j$	1	1	∞	$(v/e)^v$	No
Showalter	$\frac{1 - \exp(-\frac{\lambda}{\alpha})}{\lambda}$	1	1	∞	$(v/e)^v$	No

(ii) The filter q_α , $\alpha \in \mathcal{A}$, is called *ordered*, if further the sequence $\{q_\alpha(\lambda_k)\}_{k=1}^\infty$ is strictly monotone, i.e.

$$\alpha_1 > \alpha_2 \quad \Rightarrow \quad \forall k \in \mathbb{N}: \quad q_{\alpha_1}(\lambda_k) \leq q_{\alpha_2}(\lambda_k) \quad \text{and} \quad \exists k_0 \in \mathbb{N}: \quad q_{\alpha_1}(\lambda_{k_0}) < q_{\alpha_2}(\lambda_{k_0}),$$

and continuous as $\mathcal{A} \ni \alpha \mapsto \{q_\alpha(\lambda_k)\}_{k=1}^\infty \in \ell^2$.

The requirement of an ordered filter is rather weak, as it is satisfied by various regularization methods. In Table 1 we give several examples of such. Note that for spectral cut-off regularization, the set \mathcal{A} has to be chosen as $\{\lambda_k : k = 1, 2, \dots\} \cup \{0\}$ in order to guarantee the strict monotonicity and the continuity required by condition (ii) in Definition 1. In Table 1 we also indicate whether the method can be implemented without SVD. This property is extremely crucial in practice, especially for large-scale applications, where the computation of an SVD is often impossible given limited time and resources. The implementation of Showalter's method, for instance, can avoid SVD by employing Runge–Kutta schemes, see e.g. Rieder [54]. For a further discussion of these and other methods we refer to the monograph by Engl et al. [22].

In this paper, we focus on the asymptotic properties of ordered filter based regularization methods as the noise level σ goes to zero. As noticed by Bakushinskiĭ [2], the convergence rate of any regularization method can be arbitrarily slow if the underlying problem is ill-posed. In order to derive convergence rates we need to assume some smoothness about the unknown truth f . Typically, the smoothness of f is measured relative to the smoothing properties of the forward operator T in terms of a *source condition*, i.e. we assume that

$$f \in \mathcal{W}_\phi(\rho) := \{f \in \mathcal{X} : f = \phi(T^*T)w, \|w\|_{\mathcal{X}} \leq \rho\} \quad \text{for some constant } \rho, \quad (7)$$

where $\phi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is a so-called *index function*, i.e. ϕ is continuous, strictly increasing, and $\phi(0) = 0$. For any $f \in \mathcal{X}$ there exist a function $\tilde{\phi}$ and a constant $\tilde{\rho}$ such that $f \in \mathcal{W}_{\tilde{\phi}}(\tilde{\rho})$, cf. Mathé and Hofmann [45].

To take advantage of (7) we furthermore assume that ϕ is a *qualification* of the filter q_α , this is

$$\sup_{\lambda \in [0, \lambda_1]} \phi(\lambda) |1 - \lambda q_\alpha(\lambda)| \leq C_\phi \phi(\alpha) \quad \text{for all } \alpha \in \mathcal{A}, \quad (8)$$

with C_ϕ being a constant depending only on ϕ . For further details on general source conditions and corresponding qualifications we refer to Mathé and Pereverzev [47]. As an example consider $\phi(t) = t^v$, which is known as Hölder type source condition of order $v > 0$:

$$\mathcal{W}_v(\rho) := \{f \in \mathcal{X} : f = (T^*T)^v w, \|w\|_{\mathcal{X}} \leq \rho\}. \quad (9)$$

The function $\phi(t) = t^v$ is a qualification of the filter q_α if

$$\sup_{\lambda \in [0, \lambda_1]} \lambda^v |1 - \lambda q_\alpha(\lambda)| \leq C_v \alpha^v \quad \text{for all } \alpha \in \mathcal{A}. \quad (10)$$

In this case, the largest possible v such that (10) is satisfied, is called the classical or polynomial *qualification index* v_0 of the ordered filter q_α . For the methods discussed in Table 1, v_0 as well as C_v is also depicted.

For further reference, we collect the assumed properties of f and q_α as follows:

Assumption 1.

(i) The true solution f satisfies $f \in \mathcal{W}_\phi(\rho)$ as in (7).

- (ii) The function ϕ is a qualification of the filter q_α as in (8).
- (iii) The function $\psi(x) := x\phi^{-1}(\sqrt{x})$, with ϕ^{-1} being the inverse function of ϕ , is convex.

Remark 2. We stress that, being a standard assumption for convergence analysis, Assumption 1(iii) actually imposes no restriction, since one can always work on a slightly larger source set $\mathcal{W}_{\tilde{\phi}}$ with another index function $\tilde{\phi}$ for which Assumption 1(iii) is satisfied. Note that the function ψ is strictly increasing, and its range is \mathbb{R}_+ .

2.2. Empirical prediction risk minimization

As discussed in the Introduction, the optimal regularization parameter α will in general depend on Y , σ and f , but the latter is unknown and hence this α cannot be realized in practice. Recall that we always assume $\sigma > 0$ to be known. By means of the prediction risk $r(\alpha, f)$, the optimal $\alpha \in \mathcal{A}$ is given by

$$\alpha_o = \operatorname{argmin}_{\alpha \in \mathcal{A}} r(\alpha, f), \quad (11)$$

which is well-defined by similar arguments as in Appendix A. As a common remedy, we will try to estimate α_o from the observations Y in (1) by minimizing an unbiased estimator of $r(\alpha, f)$, which can be derived as follows. Let us introduce the shorthand notation

$$s_\alpha(\lambda) := \lambda q_\alpha(\lambda).$$

Then we have

$$\begin{aligned} r(\alpha, f) &= \mathbb{E}[\|T(q_\alpha(T^*T)T^*(Tf + \sigma\xi) - f)\|_{\mathcal{Y}}^2] \\ &= \|(I - Tq_\alpha(T^*T)T^*)Tf\|_{\mathcal{Y}}^2 + \sigma^2 \mathbb{E}[\|Tq_\alpha(T^*T)T^*\xi\|_{\mathcal{Y}}^2] \\ &= \sum_{k=1}^{\infty} \lambda_k (1 - s_\alpha(\lambda_k))^2 f_k^2 + \sigma^2 \sum_{k=1}^{\infty} s_\alpha(\lambda_k)^2, \end{aligned} \quad (12)$$

and furthermore

$$\begin{aligned} &\mathbb{E}[\|T\hat{f}_\alpha\|_{\mathcal{Y}}^2 - 2\langle Y, T\hat{f}_\alpha \rangle_{\mathcal{Y}^* \times \mathcal{Y}}] \\ &= \mathbb{E}[\|Tq_\alpha(T^*T)T^*(Tf + \sigma\xi)\|_{\mathcal{Y}}^2 - 2\langle Tf + \sigma\xi, Tq_\alpha(T^*T)T^*(Tf + \sigma\xi) \rangle_{\mathcal{Y}^* \times \mathcal{Y}}] \\ &= \sum_{k=1}^{\infty} \lambda_k (1 - s_\alpha(\lambda_k))^2 f_k^2 - \sum_{k=1}^{\infty} \lambda_k f_k^2 + \sigma^2 \sum_{k=1}^{\infty} s_\alpha(\lambda_k)^2 - 2\sigma^2 \sum_{k=1}^{\infty} s_\alpha(\lambda_k). \end{aligned}$$

Consequently for $\hat{r}(\alpha, Y)$ as in (3) we have

$$\mathbb{E}[\hat{r}(\alpha, Y)] = r(\alpha, f) - \sum_{k=1}^{\infty} \lambda_k f_k^2,$$

i.e. up to a constant independent of α , $\hat{r}(\alpha, Y)$ is an unbiased estimator of $r(\alpha, f)$. Hence we define

$$\alpha_{\text{pred}} = \operatorname{argmin}_{\alpha \in \mathcal{A}} \hat{r}(\alpha, Y). \quad (13)$$

Note that α_{pred} is measurable and almost surely well-defined, see Appendix A for details.

Remark 3. For the clarity of our notation, we stress that $\alpha \mapsto r(\alpha, f)$ is a deterministic function, whereas $\alpha \mapsto \hat{r}(\alpha, Y)$ is a random function and consequently, $\alpha_{\text{pred}} \equiv \alpha_{\text{pred}}(Y)$ as in (13) is a random variable. By $\mathbb{E}[\cdot]$ we always denote the expectation with respect to the data Y or equivalently the noise ξ . To obtain bounds for the estimator $\hat{f}_{\alpha_{\text{pred}}}$ we will also need bounds for $r(\alpha_{\text{pred}}, f)$, i.e. a deterministic function evaluated at a random variable. In particular, we stress that $\mathbb{E}[r(\alpha_{\text{pred}}, f)] \neq \mathbb{E}[\|T\hat{f}_{\alpha_{\text{pred}}} - Tf\|_{\mathcal{Y}}^2]$.

Note that α_{pred} is computable in practice as it only relies on the data, the forward operator and the noise level (which is assumed to be known, see Section 6 for estimated noise levels). As discussed in the Introduction, there are many results available for the performance of $\hat{f}_{\alpha_{\text{pred}}}$ measured by the prediction risk, among which the most precise one is due to Kneip [35] given below.

Theorem 2.1 (Deviation bound of prediction risk [35]). *Assume the model (1). Let $\hat{f}_\alpha = q_\alpha(T^*T)T^*Y$ with an ordered filter q_α , α_o as in (11), and α_{pred} as in (13). Then there exist universal positive constants C'_ξ, C''_ξ such that for all $x \geq 0$ and for all $f \in \mathcal{X}$,*

$$\mathbb{P}\left\{\frac{1}{\sigma^2}\|T\hat{f}_{\alpha_{\text{pred}}} - Tf\|_{\mathcal{Y}}^2 - \frac{1}{\sigma^2}\|T\hat{f}_{\alpha_o} - Tf\|_{\mathcal{Y}}^2 \geq x\right\} \leq C'_\xi \exp\left(-C''_\xi \min\left\{\sqrt{x}, \frac{x}{\sqrt{r(\alpha_o, f)/\sigma^2}}\right\}\right),$$

which remains true when replacing $\frac{1}{\sigma^2}\|T\hat{f}_{\alpha_{\text{pred}}} - Tf\|_{\mathcal{Y}}^2 - \frac{1}{\sigma^2}\|T\hat{f}_{\alpha_o} - Tf\|_{\mathcal{Y}}^2$ by $\frac{1}{\sigma^2}r(\alpha_{\text{pred}}, f) - \frac{1}{\sigma^2}r(\alpha_o, f)$.

Proof. Recall that $\dim \mathcal{X} = \infty$, which, together with the injectivity of T , implies $\dim \mathcal{Y} = \infty$. In fact, the assertion for finite dimensional \mathcal{Y} follows directly from Proposition 1(i) and Theorem 1 in [35] by chasing the dependency of the constants on the noise level σ . Concerning the key technical tools in Kneip's proof, we note that the Lemma 2 there actually holds for infinite sequences $a \in \ell^2$ and bounded linear trace operators $A : \ell^2 \rightarrow \ell^2$, and that the Lemma 3 there can be extended to infinite dimensional ordered linear smoothers, as long as they are Hilbert–Schmidt. Thus, the proof by Kneip [35] carries over to the case that $\dim \mathcal{Y} = \infty$. \square

The above theorem, in particular, implies (cf. [15, Theorem 1])

$$\mathbb{E}\left[\|T\hat{f}_{\alpha_{\text{pred}}} - Tf\|_{\mathcal{Y}}^2\right] \leq r(\alpha_o, f) + C\sigma\sqrt{r(\alpha_o, f)} \quad \text{for every } f \in \mathcal{X},$$

which guarantees the order optimality of $\hat{f}_{\alpha_{\text{pred}}}$ in terms of the prediction risk.

3. MISE estimates

The section is devoted to the convergence analysis of $\hat{f}_\alpha = q_\alpha(T^*T)T^*Y$ with $\alpha = \alpha_{\text{pred}}$ as in (13). In what follows, we will prove that $\hat{f}_{\alpha_{\text{pred}}}$ also possesses an optimality property in terms of the direct risk, i.e. the mean integrated square error (MISE).

3.1. Assumptions and merit discussions

We start with some technical assumptions. As we have already seen in the previous section, many calculations involve summations over $\{\lambda_k\}_{k=1}^\infty$, which can be formulated as Lebesgue–Stieltjes integrals with respect to

$$\Sigma(x) := \#\{k : \lambda_k \geq x\}.$$

Following Bissantz et al. [8], we assume that Σ can be approximated by a smooth function S to avoid the difficulty caused by the non-smoothness of Σ :

Assumption 2.

(i) There exists a surrogate function $S \in \mathcal{C}^2((0, \infty))$ of Σ satisfying

$$\lim_{\alpha \searrow 0} S(\alpha)/\Sigma(\alpha) = 1,$$

$$S'(\alpha) < 0 \quad \text{for all } \alpha > 0,$$

$$\lim_{\alpha \nearrow \infty} S(\alpha) = \lim_{\alpha \nearrow \infty} S'(\alpha) = 0,$$

$$\lim_{\alpha \searrow 0} \alpha S(\alpha) = 0.$$

(ii) There exist constants $\alpha_1 \in (0, \lambda_1]$ and $C_S > 0$ such that

$$\frac{1}{\alpha} \int_0^\alpha S(t) dt \leq C_S S(\alpha) \quad \text{for all } \alpha \in (0, \alpha_1].$$

(iii) There exists a constant $C_q > 0$ such that

$$\int_1^\infty \Psi'(C_q x) \exp\left(-C_\xi'' \sqrt{\frac{x}{2}}\right) dx < \infty \quad \text{with } \Psi(x) := \frac{x}{(S^{-1}(x))^2}.$$

Here C_ξ'' is as in Theorem 2.1.

Remark 4. Note that Assumption 2(ii) holds true if there exists some $\tilde{C}_S \in (0, 2)$ such that

$$-\alpha S'(\alpha) \text{ is integrable on } (0, \alpha_1], \quad \text{and} \quad \frac{S''(\alpha)}{-S'(\alpha)} \leq \frac{\tilde{C}_S}{\alpha} \quad \text{for all } \alpha \in (0, \alpha_1],$$

see Lemma 12 in [8] for a proof. Thus, Assumption 2(i) and (ii) are slightly weaker than Assumption 2 in [8] with a proper extension of S to a larger domain $(0, \infty)$. We stress that these are rather weak requirements, and cover a wide range of situations (see e.g. [8, Section 5]). The additional Assumption 2(iii) is needed to control certain general moments of $r(\alpha_{\text{pred}}, f)$ with the help of Theorem 2.1.

The next assumption concerns the choice of regularization parameter α for (ordered) filters q_α .

Assumption 3.

- (i) For $\alpha \in \mathcal{A}$, the function $\lambda \mapsto s_\alpha(\lambda)$ is non-decreasing.
- (ii) There exists $c_q > C_q^{-1/2}$ with C_q as in Assumption 2(iii) such that

$$s_\alpha(\alpha) = \alpha q_\alpha(\alpha) \geq c_q \quad \text{as } \alpha \searrow 0. \quad (14)$$

Remark 5. It is easy to see that the above condition with some $c_q > 0$ is satisfied by all the regularization methods in Table 1, which indicates that Assumption 3 is fairly general. In particular, Assumption 3(ii) can be understood as a parametrization condition. For instance, the Tikhonov method with re-parametrization $\alpha \mapsto \sqrt{\alpha}$, i.e. $q_\alpha(\lambda) = 1/(\sqrt{\alpha} + \lambda)$, still defines an ordered filter, but does not satisfy (14) anymore. The condition $c_q > C_q^{-1/2}$ requires some compatibility of the ill-posedness with the parametrization of the filter. Note that the qualification condition (8) implies that $s_\alpha(\alpha) \leq 1$ for $\alpha > 0$, so if $C_q > 1$ then the relation $c_q > C_q^{-1/2}$ is automatically satisfied.

Under these assumptions, upper bounds for \hat{f}_α with an a-priori choice of α have been proven by Bissantz et al. [8]:

Theorem 3.1 (A-priori parameter choice [8]). Consider the model (1), and let $\hat{f}_\alpha := q_\alpha(T^*T)T^*Y$ with a filter q_α , and suppose that Assumption 2(i)–(ii) holds true. Let also α_* satisfy

$$\alpha_* \phi(\alpha_*)^2 = \sigma^2 S(\alpha_*). \quad (15)$$

- (i) If Assumption 1(ii) holds, there is a constant C_1 depending only on $\rho, C_\phi, C_q', C_q''$ and C_S such that

$$\sup_{f \in \mathcal{W}_\phi(\rho)} \mathbb{E}[\|\hat{f}_{\alpha_*} - f\|_{\mathcal{X}}^2] \leq C_1 \phi(\alpha_*)^2 = C_1 \sigma^2 \frac{S(\alpha_*)}{\alpha_*} \quad \text{as } \sigma \searrow 0.$$

- (ii) If $\tilde{\phi}(t) := \sqrt{t} \phi(t)$ is a qualification of the filter q_α , namely,

$$\sup_{\lambda \in [0, \lambda_1]} \tilde{\phi}(\lambda) |1 - \lambda q_\alpha(\lambda)| \leq C_\tilde{\phi} \tilde{\phi}(\alpha) \quad \text{for all } \alpha \in \mathcal{A}, \quad (16)$$

then there is a constant C_2 depending only on $\rho, C_\tilde{\phi}, C_q', C_q''$ and C_S such that

$$\sup_{f \in \mathcal{W}_\phi(\rho)} \mathbb{E}[\|T \hat{f}_{\alpha_*} - T f\|_{\mathcal{Y}}^2] \leq C_2 \alpha_* \phi(\alpha_*)^2 = C_2 \sigma^2 S(\alpha_*) \quad \text{as } \sigma \searrow 0.$$

Remark 6. Actually, the upper bounds on the risk in Theorem 3.1 consist of a bias part and a variance part. The front constant in the bias part depends only on ρ and C_ϕ (or $C_{\tilde{\phi}}$), while that in the variance part depends only on C'_q , C''_q and C_S . Moreover, it is worth noting that (16) in particular implies (8), i.e., whenever $\tilde{\phi}(t) := \sqrt{t}\phi(t)$ is a qualification of the filter q_α , then also ϕ is a qualification of the filter q_α and Assumption 1(ii) is satisfied.

3.2. Oracle inequality

We are now in position to derive an oracle inequality in the general form of (4) for the empirical parameter choice $\alpha = \alpha_{\text{pred}}$.

Theorem 3.2 (Oracle inequality). *Assume the model (1). Let $\hat{f}_\alpha := q_\alpha(T^*T)T^*Y$ with an ordered filter q_α , and Assumptions 1, 2 and 3 hold. Let also α_o be given by (11), and α_{pred} by (13). Then there are positive constants C_1 , C_2 and C_3 , independent of f , α and σ , such that*

$$\mathbb{E}[\|\hat{f}_{\alpha_{\text{pred}}} - f\|_{\mathcal{X}}^2] \leq \rho^2 \psi^{-1}\left(\sigma^2\left(\frac{2}{\rho^2}\gamma_\sigma + C_1\right)\right) + \sigma^2 C_3 \left(\frac{\gamma_\sigma + \sqrt{\gamma_\sigma}}{S^{-1}(2C_q\gamma_\sigma)} + C_2\right) \quad \text{with } \gamma_\sigma := \frac{r(\alpha_o, f)}{\sigma^2}. \quad (17)$$

Remark 7. Despite the fact that (17) is not an oracle inequality in the strict sense as discussed e.g. by [12], we still call (17) an oracle inequality as it relates the direct risk under α_{pred} with the weak oracle risk $r(\alpha_o, f)$. We emphasize that this is in line with [15] and refer to [62] for further discussion. Moreover, we point out that constants C_1 , C_2 in Theorem 3.2 are in fact universal, while C_3 depends only on C'_q , C''_q , C_q , C_S , c_q and the operator T .

The proof of Theorem 3.2 is based on a general strategy together with technical lemmata, and is postponed to Section 4. To ease the understanding of this paper, we will now start with conclusions from Theorem 3.2.

3.3. Convergence rates and examples

The derived oracle inequality in Theorem 3.2 readily provides error estimates for the estimator $\hat{f}_{\alpha_{\text{pred}}}$ given proper upper bounds of the oracle prediction risk $r(\alpha_o, f)$ as in Theorem 3.1.

Theorem 3.3 (Convergence rates). *Assume the same setting as in Theorem 3.2, and additionally that $\tilde{\phi}(t) = \sqrt{t}\phi(t)$ is a qualification of the filter q_α . Let α_* be given by (15). Then as $\sigma \searrow 0$ we have*

$$\sup_{f \in \mathcal{W}_{\tilde{\phi}}(\rho)} \mathbb{E}[\|\hat{f}_{\alpha_{\text{pred}}} - f\|_{\mathcal{X}}^2] \leq C_1 \phi(\alpha_*)^2 + C_3 \frac{\alpha_* \phi(\alpha_*)^2}{S^{-1}(C_2 C_q \frac{\alpha_* \phi(\alpha_*)^2}{\sigma^2})} = C_1 \sigma^2 \frac{S(\alpha_*)}{\alpha_*} + C_3 \frac{\sigma^2 S(\alpha_*)}{S^{-1}(C_2 C_q S(\alpha_*))}$$

for some constants $C_1, C_2, C_3 > 0$ independent of σ .

Proof. From Theorem 3.2, it follows that

$$\sup_{f \in \mathcal{W}_{\tilde{\phi}}(\rho)} \mathbb{E}[\|\hat{f}_{\alpha_{\text{pred}}} - f\|_{\mathcal{X}}^2] \leq \sup_{f \in \mathcal{W}_{\tilde{\phi}}(\rho)} \left(\rho^2 \psi^{-1}\left(\frac{2}{\rho^2} r(\alpha_o, f) + C_1 \sigma^2\right) + C_3 \left(\frac{r(\alpha_o, f) + \sigma \sqrt{r(\alpha_o, f)}}{S^{-1}(2C_q \frac{r(\alpha_o, f)}{\sigma^2})} + C_2 \sigma^2\right) \right),$$

where C_1, C_2 are universal, and C_3 depends only on $C'_q, C''_q, C_q, C_S, c_q$ and the operator T . By Theorem 3.1(ii), there is a constant $C_4 \geq \rho^2$ depending only on $\rho, C_{\tilde{\phi}}, C'_q, C''_q$ and C_S such that

$$\sup_{f \in \mathcal{W}_{\tilde{\phi}}(\rho)} r(\alpha_o, f) \leq \sup_{f \in \mathcal{W}_{\tilde{\phi}}(\rho)} r(\alpha_*, f) \leq C_4 \alpha_* \phi(\alpha_*)^2 = C_4 \sigma^2 S(\alpha_*) \quad \text{for sufficiently small } \sigma.$$

Note that by definition $\alpha_* \searrow 0$ as $\sigma \searrow 0$, so

$$\frac{\alpha_* \phi(\alpha_*)^2}{\sigma^2} = S(\alpha_*) \nearrow \infty \quad \text{as } \sigma \searrow 0.$$

Recall that $\psi(x) = x\phi^{-1}(\sqrt{x})$ is strictly increasing and convex, and $\psi(0) = 0$. Thus, ψ^{-1} is strictly increasing, and $\psi^{-1}(cx) \leq c\psi^{-1}(x)$ for any $c \geq 1$. Note also that S^{-1} is strictly decreasing. Thus, for small enough σ

$$\begin{aligned} & \rho^2 \psi^{-1} \left(\frac{2}{\rho^2} r(\alpha_o, f) + C_1 \sigma^2 \right) + C_3 \left(\frac{r(\alpha_o, f) + \sigma \sqrt{r(\alpha_o, f)}}{S^{-1}(2C_q \frac{r(\alpha_o, f)}{\sigma^2})} + C_2 \sigma^2 \right) \\ & \leq \rho^2 \psi^{-1} \left(\frac{3}{\rho^2} C_4 \alpha_* \phi(\alpha_*)^2 \right) + \frac{2C_3 C_4 \alpha_* \phi(\alpha_*)^2}{S^{-1}(2C_q C_4 \frac{\alpha_* \phi(\alpha_*)^2}{\sigma^2})} \\ & \leq 3C_4 \psi^{-1}(\alpha_* \phi(\alpha_*)^2) + \frac{2C_3 C_4 \alpha_* \phi(\alpha_*)^2}{S^{-1}(2C_q C_4 \frac{\alpha_* \phi(\alpha_*)^2}{\sigma^2})} = 3C_4 \phi(\alpha_*)^2 + \frac{2C_3 C_4 \alpha_* \phi(\alpha_*)^2}{S^{-1}(2C_q C_4 \frac{\alpha_* \phi(\alpha_*)^2}{\sigma^2})}, \end{aligned}$$

which holds uniformly over $f \in \mathcal{W}_\phi(\rho)$, and thus concludes the proof. \square

Remark 8. If, in addition, there is a constant $\tilde{C} > 0$ such that

$$S(\tilde{C}x) \geq C_2 C_q S(x) \quad \text{for all } x > 0,$$

then it follows from Theorem 3.3 that

$$\sup_{f \in \mathcal{W}_\phi(\rho)} \mathbb{E}[\|\hat{f}_{\alpha_{\text{pred}}} - f\|_{\mathcal{X}}^2] \leq C \phi(\alpha_*)^2 = C \sigma^2 \frac{S(\alpha_*)}{\alpha_*}$$

with some $C > 0$ independent of α_* and σ . This coincides with the convergence rate we obtain under an a-priori parameter choice in Theorem 3.1, which turns out to be order optimal in most cases, see e.g. Section 3.3.1 and Bissantz et al. [8].

We note that there are two additional important assumptions for a-posteriori parameter choice α_{pred} compared to the a-priori choice (cf. Theorem 3.1(i) and Theorem 3.3). The one is Assumption 2(iii), which concerns the control of general moments of $r(\alpha_{\text{pred}}, f)$, due to the randomness of α_{pred} . The other is that not only ϕ but also $\tilde{\phi}(t) = \sqrt{t}\phi(t)$ is a qualification of the filter q_α . The latter seems to be typical for parameter choice rule relying on residuals in image space, as e.g. for the discrepancy principle in case of deterministic inverse problems, see Engl et al. [22, Section 4.3] and Mathé and Pereverzev [48], or for generalized cross-validation (GCV), see Lukas [40] and Vogel [58]. Still we stress that the qualification assumption plays no role in the proof of the oracle inequality (Theorem 3.2), and it only kicks in for the derivation of convergence rates for $\hat{f}_{\alpha_{\text{pred}}}$ through $r(\alpha_o, f)$ in the convergence analysis under the a-priori parameter choice.

3.3.1. Mildly ill-posed problems

We now consider a particular mildly ill-posed problem. More precisely, we assume

Assumption 4.

(i) Polynomial decay of eigenvalues of T^*T

$$\lambda_k = C_a k^{-a}, \quad k = 1, 2, \dots \text{ with some } a > 1 \text{ and } C_a > 0.$$

(ii) Smoothness of the truth

$$f \in \mathcal{S}_b := \left\{ f \in \mathcal{X} : \sum_{k=1}^{\infty} w_k f_k^2 \leq 1 \right\} \quad \text{with } w_k = C_b k^b, k = 1, 2, \dots,$$

for some positive constants b and C_b .

In the above assumption, the requirement of $a > 1$ is to ensure that the forward operator T is Hilbert–Schmidt, and the smoothness class \mathcal{S}_b is equivalent to the Hölder type source condition of order $b/(2a)$, more precisely, $\mathcal{S}_b \equiv \mathcal{W}_{b/(2a)}(C_a^{-b/a} C_b^{-1})$ in (9).

In this simple setting the convergence rates of ordered filter based methods with empirical parameter choice α_{pred} can be explicitly computed.

Corollary 3.4 (Order optimality). *Assume the model (1). Let $\hat{f}_\alpha := q_\alpha(T^*T)T^*Y$ with an ordered filter q_α , and Assumptions 3 and 4 with any $c_q > 0$ hold. If the qualification index v_0 in (10) of the ordered filter satisfies $v_0 \geq b/(2a) + 1/2$, then there are positive constants C_1 and C_2 independent of σ such that*

$$\sup_{f \in \mathcal{S}_b} \mathbb{E}[\|\hat{f}_{\alpha_{\text{pred}}} - f\|_{\mathcal{X}}^2] \leq C_1 \inf_{\hat{f}} \sup_{f \in \mathcal{S}_b} \mathbb{E}[\|\hat{f} - f\|_{\mathcal{X}}^2] \leq C_2 \sigma^{\frac{2b}{a+b+1}} \quad \text{as } \sigma \searrow 0.$$

The infimum above is taken over all possible estimators \hat{f} (including both linear and nonlinear ones).

Proof. Note that $\phi(x) = x^{b/(2a)}$ and then $\psi(x) = x\phi^{-1}(\sqrt{x}) = x^{(a+b)/b}$, so Assumption 1 is satisfied. Define $S(\alpha) := (\alpha/C_a)^{-1/a}$. Elementary calculation shows that $S(\alpha)$ satisfies Assumption 2(i) and (ii). Since $\Psi(x) = x/(S^{-1}(x))^2 = C_a^{-2}x^{1+2a}$, Assumption 2(iii) clearly holds. By definition (15), it follows that $\alpha_* = C_a^{1/(1+a+b)}\sigma^{2a/(1+a+b)}$. Thus, by Theorem 3.3 and Remark 8, we have

$$\sup_{f \in \mathcal{S}_b} \mathbb{E}[\|\hat{f}_{\alpha_{\text{pred}}} - f\|_{\mathcal{X}}^2] \leq C_1 \phi(\alpha_*)^2 = C_1 C_a^{\frac{b}{a(1+a+b)}} (\sigma^2)^{\frac{b}{1+a+b}} \quad \text{as } \sigma \searrow 0,$$

for some positive constant C_1 .

Further, it is well-known (see e.g. [20,25,52])

$$\inf_{\hat{f}} \sup_{f \in \mathcal{S}_b} \mathbb{E}[\|\hat{f} - f\|_{\mathcal{X}}^2] \geq C_2 (\sigma^2)^{\frac{b}{a+b+1}} \quad \text{for some } C_2 > 0.$$

This concludes the proof. □

Remark 9. The above proposition in particular implies that all the methods in Table 1 are order optimal with $\alpha = \alpha_{\text{pred}}$ when $b/(2a) + 1/2 \leq v_0$ in the minimax sense. This reproduces the result in Chernousova and Golubev [15] for the spectral cut-off method as a special case.

Note that the parameter choice α_{pred} depends only on the data, and is completely independent of the unknown truth. Thus, the ordered filter based regularization methods with α_{pred} automatically adapt to the unknown smoothness of the truth, and achieve the best possible rates up to a constant. In other words, the ordered filter based regularization methods with parameter choice α_{pred} are *adaptively minimax optimal* (cf. [52]) over a range of smoothness classes, and the adaptation range is determined by the qualification index of the filter and the smoothing property of the forward operator. Importantly, we point out that the order optimality here is in sharp contrast to the Lepskii-type balancing principle [36], where one typically loses a log-factor in the asymptotic convergence rates.

In addition, we stress again the price we pay for a-posteriori parameter choice α_{pred} is a stronger qualification assumption $b/(2a) + 1/2 \leq v_0$, as the convergence rates of direct risk for a-priori parameter choice only asks for $b/(2a) \leq v_0$ by Theorem 3.1(i), see also Remark 8.

3.3.2. Exponentially ill-posed problems

Next we consider an exponentially ill-posed setting: The eigenvalues of T^*T satisfy

$$\lambda_k \asymp \exp(-\mu k^a), \quad k = 1, 2, \dots \text{ for some } a, \mu > 0,$$

and the smoothness of the truth is characterized by (7) with

$$\phi(x) := x^b(-\log x)^c \quad \text{for some } b > 0, c \in \mathbb{R}, \text{ or } b = 0, c > 0.$$

That is, we assume that the truth lies in $\{f \in \mathcal{X} : \sum_{k=1}^{\infty} w_k f_k^2 \leq 1\}$ with $w_k \asymp k^{-2ac} \exp(2\mu b k^a)$.

It is easy to see that the assumptions of Theorem 3.2 are satisfied for all the regularization methods listed in Table 1 provided that $0 < a < 1/2$, or $a = 1/2$ and μ is sufficiently small. Hence, if in addition $b + 1/2 < v_0$, or $b = v_0$, $c \leq 0$ (recall that v_0 is the qualification index), we can obtain certain error bounds by means of Theorem 3.3. However, it turns out that our bounds are too rough to guarantee order optimality. In fact, in case of $b = 0$, the error bound on the right-hand side of (17) even diverges as the noise level σ tends to 0. In summary, our oracle inequality is applicable for exponentially ill-posed problems as discussed here, but is not strong enough to derive rates of convergence or even show optimality of the investigated parameter choice α_{pred} . We refer to [62] for numerical simulations in exponentially ill-posed examples, in the view of which it seems questionable if the parameter choice rule under investigation still yields optimal results, being in line with the findings by Lucka et al. [38].

4. A general methodology for proving the oracle inequality

To prove our oracle inequality (17), we will proceed as follows. First, we obtain bounds for general moments of the prediction risk (cf. Corollary 4.1). Secondly, we proceed with a standard estimate for the (deterministic) bias of the estimator \hat{f}_α under the smoothness Assumption 1 (cf. Lemma 4.2). Finally, we prove a comparison lemma on the variance terms (cf. Lemma 4.3). Putting these three ingredients together, the proof of Theorem 3.2 is then straightforward. More importantly, we stress that, if these three ingredients are given for some parameter choice rule $\tilde{\alpha}$, an oracle inequality similar to (17) can be derived.

4.1. Main ingredients

We start with bounds for general moments of the prediction risk.

Corollary 4.1 (General moments of prediction risk). *Assume the same setting as Theorem 2.1, and let $\Psi : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ be an increasing and continuously differentiable function with $\Psi(0) = 0$ such that*

$$C_\Psi := C'_\xi \int_0^\infty \Psi'(x) \exp\left(-C''_\xi \sqrt{\frac{x}{2}}\right) dx < \infty \quad (18)$$

with C'_ξ, C''_ξ being the same as in Theorem 2.1. Then

$$\mathbb{E}\left[\Psi\left(\frac{r(\alpha_{\text{pred}}, f)}{\sigma^2}\right)\right] \leq \Psi\left(\frac{2r(\alpha_o, f)}{\sigma^2}\right) + C_\Psi \quad \text{for all } f \in \mathcal{X}.$$

Proof. Let $\gamma_\sigma := r(\alpha_o, f)/\sigma^2$ as in (17). Then

$$\begin{aligned} \mathbb{E}\left[\Psi\left(\frac{r(\alpha_{\text{pred}}, f)}{\sigma^2}\right)\right] &= \int_0^\infty \Psi'(x) \mathbb{P}\left\{\frac{r(\alpha_{\text{pred}}, f)}{\sigma^2} \geq x\right\} dx && \text{[by Fubini's theorem]} \\ &\leq \int_0^{2\gamma_\sigma} \Psi'(x) dx + C'_\xi \int_{2\gamma_\sigma}^\infty \Psi'(x) \exp(-C''_\xi \sqrt{x - \gamma_\sigma}) dx && \text{[by Theorem 2.1]} \\ &\leq \Psi(2\gamma_\sigma) + C'_\xi \int_{2\gamma_\sigma}^\infty \Psi'(x) \exp\left(-C''_\xi \sqrt{\frac{x}{2}}\right) dx \\ &\leq \Psi\left(\frac{2r(\alpha_o, f)}{\sigma^2}\right) + C_\Psi. \end{aligned}$$

This concludes the proof. \square

Remark 10. A simple example is $\Psi(x) := x^\theta$ for some $\theta > 0$. By Corollary 4.1, it leads to

$$\mathbb{E}[r(\alpha_{\text{pred}}, f)^\theta] \leq 2^\theta r(\alpha_o, f)^\theta + C_\theta \sigma^{2\theta},$$

where the second term on the right hand side is typically negligible compared to the first as σ tends to 0. Note that condition (18) only requires

$$\int_c^\infty \Psi'(x) \exp\left(-C''_\xi \sqrt{\frac{x}{2}}\right) dx < \infty \quad \text{for some constant } c > 0.$$

Based on the smoothness Assumption 1, we can prove the following estimate for the bias of \hat{f}_α :

Lemma 4.2 (Source condition). *Under Assumption 1(i) and (iii), it holds that*

$$\sum_{k=1}^\infty (1 - s_\alpha(\lambda_k))^2 f_k^2 \leq \rho^2 \psi^{-1}\left(\frac{1}{\rho^2} \sum_{k=1}^\infty \lambda_k (1 - s_\alpha(\lambda_k))^2 f_k^2\right),$$

with ρ as in (7).

Proof. Based on spectral analysis, condition (7) can be equivalently written as

$$f_k = \phi(\lambda_k)w_k, \quad k = 1, 2, \dots, \text{ with } \sum_{k=1}^{\infty} w_k^2 \leq \rho^2.$$

Thus, $f_k^2 \leq \rho^2 \phi(\lambda_k)^2$ and then $\phi^{-1}(\sqrt{\rho^{-2} f_k^2}) \leq \lambda_k$. Note that $\psi(0) = 0$ and $\psi(cx) \geq c\psi(x)$ for any $c \geq 1$. By the convexity of ψ and Jensen's inequality, we have for any $n \in \mathbb{N}$

$$\begin{aligned} \psi\left(\sum_{k=1}^n \rho^{-2} f_k^2 (1 - s_\alpha(\lambda_k))^2\right) &\leq \psi\left(\sum_{k=1}^n \rho^{-2} f_k^2 \frac{(1 - s_\alpha(\lambda_k))^2}{1 + \sum_{i=1}^n (1 - s_\alpha(\lambda_i))^2}\right) \left(1 + \sum_{i=1}^n (1 - s_\alpha(\lambda_i))^2\right) \\ &\leq \sum_{k=1}^n \psi(\rho^{-2} f_k^2) \frac{(1 - s_\alpha(\lambda_k))^2}{1 + \sum_{i=1}^n (1 - s_\alpha(\lambda_i))^2} \left(1 + \sum_{i=1}^n (1 - s_\alpha(\lambda_i))^2\right) \\ &= \sum_{k=1}^n \psi(\rho^{-2} f_k^2) (1 - s_\alpha(\lambda_k))^2 \leq \rho^{-2} \sum_{k=1}^n \lambda_k f_k^2 (1 - s_\alpha(\lambda_k))^2 \\ &\leq \rho^{-2} \sum_{k=1}^{\infty} \lambda_k f_k^2 (1 - s_\alpha(\lambda_k))^2. \end{aligned}$$

The assertion follows by applying ψ^{-1} to the above inequality and letting $n \nearrow \infty$. □

Finally, we need certain comparison relations, which are used for bounding the variance part of the risk:

Lemma 4.3 (Comparison). *Let q_α be a filter, and Assumptions 2 and 3 hold. Then there are positive constants C_1 and C_2 , depending only on $C'_q, C''_q, C_q, C_S, c_q$ and the operator T , such that for every $\alpha \in \mathcal{A}$*

$$\sum_{k=1}^{\infty} \lambda_k q_\alpha(\lambda_k)^2 \leq C_1 \Psi_1\left(C_q \sum_{k=1}^{\infty} s_\alpha(\lambda_k)^2\right) \quad \text{and} \quad \sum_{k=1}^{\infty} \lambda_k^2 q_\alpha(\lambda_k)^4 \leq C_2 \Psi_2\left(C_q \sum_{k=1}^{\infty} s_\alpha(\lambda_k)^2\right),$$

with C'_q, C''_q in Definition 1, C_q, C_S in Assumption 2, c_q in Assumption 3, and functions Ψ_1 and Ψ_2 by

$$\Psi_1(x) := \frac{x}{S^{-1}(x)}, \quad \Psi_2(x) := \frac{x}{(S^{-1}(x))^2}, \quad \text{for every } x > 0. \quad (19)$$

Proof. By Assumptions 2(i) and 3(ii), and $c_q^2 C_q > 1$, there are $\alpha_0, \alpha_1 \in (0, \min\{1, \alpha_1\})$, with α_1 in Assumption 2(ii), and some constant $\delta \in (0, 1)$ such that for every $\alpha \leq \alpha_0$ it holds that

$$s_\alpha(\alpha) \geq \delta c_q, \quad \text{and} \quad \frac{1}{\delta^2 c_q^2 C_q} \leq \frac{\Sigma(\alpha)}{S(\alpha)} \leq 2. \quad (20)$$

We consider two separate cases:

Case I: $\alpha \leq \alpha_0$. Then

$$\begin{aligned} \sum_{k=1}^{\infty} s_\alpha(\lambda_k)^2 &= - \int_0^\infty t^2 q_\alpha(t)^2 d\Sigma(t) \geq - \int_\alpha^\infty t^2 q_\alpha(t)^2 d\Sigma(t) \\ &\geq - \int_\alpha^\infty \alpha^2 q_\alpha(\alpha)^2 d\Sigma(t) && \text{[by Assumption 3(i)]} \\ &\geq -\delta^2 c_q^2 \int_\alpha^\infty d\Sigma(t) = \delta^2 c_q^2 \Sigma(\alpha) && \text{[by (20)]} \\ &\geq \frac{1}{C_q} S(\alpha). && \text{[by (20)]} \end{aligned} \quad (21)$$

Denote $\tilde{C}_q := \max\{C'_q, C''_q\}$. Then

$$\begin{aligned}
\sum_{k=1}^{\infty} \lambda_k q_\alpha(\lambda_k)^2 &= - \int_0^\infty t q_\alpha(t)^2 d\Sigma(t) \\
&\leq \tilde{C}_q^2 \left(- \int_0^\alpha \frac{t}{\alpha^2} d\Sigma(t) - \int_\alpha^\infty \frac{1}{t} d\Sigma(t) \right) && \text{[by Definition 1(i)]} \\
&\leq \tilde{C}_q^2 \left(- \frac{t}{\alpha^2} \Sigma(t) \Big|_0^\alpha + \frac{1}{\alpha^2} \int_0^\alpha \Sigma(t) dt + \frac{1}{\alpha} \Sigma(\alpha) \right) = \frac{\tilde{C}_q^2}{\alpha^2} \int_0^\alpha \Sigma(t) dt \\
&\leq \frac{2\tilde{C}_q^2}{\alpha^2} \int_0^\alpha S(t) dt && \text{[by (20)]} \\
&\leq 2\tilde{C}_q^2 C_S \frac{S(\alpha)}{\alpha}, && \text{[by Assumption 2(ii)]}
\end{aligned}$$

and similarly

$$\begin{aligned}
\sum_{k=1}^{\infty} \lambda_k^2 q_\alpha(\lambda_k)^4 &= - \int_0^\infty t^2 q_\alpha(t)^4 d\Sigma(t) \\
&\leq \tilde{C}_q^4 \left(- \int_0^\alpha \frac{t^2}{\alpha^4} d\Sigma(t) - \int_\alpha^\infty \frac{1}{t^2} d\Sigma(t) \right) && \text{[by Definition 1(i)]} \\
&\leq \tilde{C}_q^4 \left(- \frac{t^2}{\alpha^4} \Sigma(t) \Big|_0^\alpha + \frac{1}{\alpha^4} \int_0^\alpha 2t \Sigma(t) dt + \frac{1}{\alpha^2} \Sigma(\alpha) \right) \\
&\leq \frac{2\tilde{C}_q^4}{\alpha^3} \int_0^\alpha \Sigma(t) dt \leq \frac{4\tilde{C}_q^4}{\alpha^3} \int_0^\alpha S(t) dt && \text{[by (20)]} \\
&\leq 4\tilde{C}_q^4 C_S \frac{S(\alpha)}{\alpha^2}. && \text{[by Assumption 2(ii)]}
\end{aligned}$$

These together with (21) prove the assertion if $\alpha \leq \alpha_0$.

Case II: $\alpha > \alpha_0$. Then by Assumption 3 it holds that

$$\sum_{k=1}^{\infty} s_\alpha(\lambda_k)^2 \geq \sum_{k=1}^{\infty} s_{\alpha_0}(\lambda_k)^2, \quad \text{a constant} \in \mathbb{R}_+.$$

By Definition 1(i) we have

$$\begin{aligned}
\sum_{k=1}^{\infty} \lambda_k q_\alpha(\lambda_k)^2 &\leq \frac{(C'_q)^2}{\alpha^2} \sum_{k=1}^{\infty} \lambda_k \leq \frac{(C'_q)^2}{\alpha_0^2} \text{Trace}(T^*T), \quad \text{and} \\
\sum_{k=1}^{\infty} \lambda_k^2 q_\alpha(\lambda_k)^4 &\leq \frac{C''_q (C'_q)^3}{\alpha^3} \sum_{k=1}^{\infty} \lambda_k \leq \frac{C''_q (C'_q)^3}{\alpha_0^3} \text{Trace}(T^*T),
\end{aligned}$$

where both upper bounds are constants in \mathbb{R}_+ . Thus, the assertion clearly holds for $\alpha > \alpha_0$.

Combining the above two cases concludes the proof. \square

4.2. Proof of Theorem 3.2

Now we are in position to prove Theorem 3.2. To obtain bounds, we will split the variance part by exploiting a technique from Golubev [27] dealing with ordered processes:

Lemma 4.4 (Ordered processes [27]). Assume that we are given a sequence of functions $c_k : \mathcal{A} \rightarrow \mathbb{R}$, $k = 1, 2, \dots$, with $\mathcal{A} \subseteq \mathbb{R}_+$, satisfying $\sum_{k=1}^{\infty} |c_k(\alpha)| < \infty$ and

$$\kappa(\alpha) := \left(\sum_{k=1}^{\infty} c_k(\alpha)^2 \right)^{1/2} < \infty \quad \text{for } \alpha \in \mathcal{A},$$

and that κ is continuous and strictly monotone on \mathcal{A} . Define $(x)_+ := \max\{x, 0\}$ and

$$\zeta(\alpha) := \sum_{k=1}^{\infty} c_k(\alpha) (\xi_k^2 - 1) \quad \text{with } \xi_k \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1).$$

Then there exists a universal constant C_ξ such that

$$\mathbb{E} \left[\sup_{\alpha \in \mathcal{A}} (\zeta(\alpha) - x\kappa(\alpha)^2)_+ \right] \leq \frac{C_\xi}{x} \quad \text{for all } x > 0.$$

Proof. Note that $\zeta(\alpha)$ is almost surely finite by means of Chebyshev's inequality and the fact that $\text{Var}[\zeta(\alpha)] = 2\kappa(\alpha) < \infty$ (or alternatively, by Kolmogorov's three-series theorem). In the terminology of Golubev [27], $\zeta(\alpha)$ is an ordered process. The assertion can be proven in exactly the same way as Lemmata 1 and 2 by [27]. \square

Proof of Theorem 3.2. Consider the bias-variance decomposition

$$\begin{aligned} \mathbb{E} [\| \hat{f}_{\alpha_{\text{pred}}} - f \|_{\mathcal{X}}^2] &\leq 2\mathbb{E} [\| (q_{\alpha_{\text{pred}}} (T^*T) T^*T - I) f \|_{\mathcal{X}}^2] + 2\sigma^2 \mathbb{E} [\| q_{\alpha_{\text{pred}}} (T^*T) T^* \xi \|_{\mathcal{X}}^2] \\ &= 2\mathbb{E} \left[\sum_{k=1}^{\infty} (1 - s_{\alpha_{\text{pred}}}(\lambda_k))^2 f_k^2 \right] + 2\sigma^2 \mathbb{E} \left[\sum_{k=1}^{\infty} \lambda_k q_{\alpha_{\text{pred}}}(\lambda_k)^2 \xi_k^2 \right]. \end{aligned} \quad (22)$$

For the first term (i.e. bias part) in (22), we have for all $f \in \mathcal{W}_\phi(\rho)$

$$\begin{aligned} \mathbb{E} \left[\sum_{k=1}^{\infty} f_k^2 (1 - s_{\alpha_{\text{pred}}}(\lambda_k))^2 \right] &\leq C_1 \mathbb{E} \left[\psi^{-1} \left(\frac{1}{C_1} \sum_{k=1}^{\infty} \lambda_k (1 - s_{\alpha_{\text{pred}}}(\lambda_k))^2 f_k^2 \right) \right] \quad [\text{by Lemma 4.2}] \\ &\leq C_1 \mathbb{E} \left[\psi^{-1} \left(\frac{1}{C_1} r(\alpha_{\text{pred}}, f) \right) \right] \quad [\text{by (12)}] \\ &\leq C_1 \psi^{-1} \left(\frac{1}{C_1} \mathbb{E} [r(\alpha_{\text{pred}}, f)] \right) \quad [\text{by Jensen's inequality}] \\ &\leq C_1 \psi^{-1} \left(\frac{2}{C_1} r(\alpha_o, f) + C_2 \sigma^2 \right), \quad [\text{by Remark 10}] \end{aligned}$$

where $C_1 := \rho^2$ with ρ in (7), and C_2 is a universal constant.

For the second term (i.e. variance part) in (22), we further split it into two terms

$$\sigma^2 \mathbb{E} \left[\sum_{k=1}^{\infty} \lambda_k q_{\alpha_{\text{pred}}}(\lambda_k)^2 \xi_k^2 \right] = \sigma^2 \mathbb{E} \left[\sum_{k=1}^{\infty} \lambda_k q_{\alpha_{\text{pred}}}(\lambda_k)^2 \right] + \sigma^2 \mathbb{E} \left[\sum_{k=1}^{\infty} \lambda_k q_{\alpha_{\text{pred}}}(\lambda_k)^2 (\xi_k^2 - 1) \right]. \quad (23)$$

Note that $\Psi_1'(x) \leq S^{-1}(x) \Psi_2'(x)$ for functions Ψ_1 and Ψ_2 in (19), so by monotonicity of S and Assumption 2(iii), condition (18) is satisfied with $\Psi(x) = \Psi_1(C_q x)$ as well. Then, for the first term in (23), it holds that

$$\begin{aligned} \sigma^2 \mathbb{E} \left[\sum_{k=1}^{\infty} \lambda_k q_{\alpha_{\text{pred}}}(\lambda_k)^2 \right] &\leq C_3 \sigma^2 \mathbb{E} \left[\Psi_1 \left(C_q \sum_{k=1}^{\infty} s_{\alpha_{\text{pred}}}(\lambda_k)^2 \right) \right] \quad [\text{by Lemma 4.3}] \\ &\leq C_3 \sigma^2 \mathbb{E} \left[\Psi_1 \left(C_q \frac{r(\alpha_{\text{pred}}, f)}{\sigma^2} \right) \right] \quad [\text{by (12)}] \end{aligned}$$

$$\begin{aligned}
&\leq C_3\sigma^2\left(\Psi_1\left(2C_q\frac{r(\alpha_o, f)}{\sigma^2}\right) + C_4\right) \quad [\text{by Corollary 4.1}] \\
&= 2C_3C_q\frac{r(\alpha_o, f)}{S^{-1}(2C_q\frac{r(\alpha_o, f)}{\sigma^2})} + C_3C_4\sigma^2,
\end{aligned}$$

where constant C_3 depends only on $C'_q, C''_q, C_q, C_S, c_q$ and the operator T , and constant C_4 is universal.

For the second term in (23), we apply Lemma 4.4 with $c_k(\alpha) = \lambda_k q_\alpha(\lambda_k)^2$, which leads to

$$\begin{aligned}
\sigma^2\mathbb{E}\left[\sum_{k=1}^{\infty}\lambda_k q_{\alpha_{\text{pred}}}(\lambda_k)^2(\xi_k^2 - 1)\right] &\leq \sigma^2\mathbb{E}[(\zeta(\alpha_{\text{pred}}) - x\kappa(\alpha_{\text{pred}})^2)_+] + \sigma^2\mathbb{E}[x\kappa(\alpha_{\text{pred}})^2] \\
&\leq \sigma^2\mathbb{E}\left[\sup_{\alpha\in\mathcal{A}}(\zeta(\alpha) - x\kappa(\alpha)^2)_+\right] + \sigma^2\mathbb{E}[x\kappa(\alpha_{\text{pred}})^2] \\
&\leq \sigma^2\frac{C_5}{x} + x\sigma^2\mathbb{E}\left[\sum_{k=1}^{\infty}\lambda_k^2 q_{\alpha_{\text{pred}}}(\lambda_k)^4\right] \quad \text{for all } x > 0,
\end{aligned}$$

where C_5 is a universal constant, and ζ and κ are defined in Lemma 4.4.

We minimize the right hand side of the above equation over $x > 0$, and then obtain

$$\begin{aligned}
\sigma^2\mathbb{E}\left[\sum_{k=1}^{\infty}\lambda_k q_{\alpha_{\text{pred}}}(\lambda_k)^2(\xi_k^2 - 1)\right] &\leq 2\sigma^2\left(C_5\mathbb{E}\left[\sum_{k=1}^{\infty}\lambda_k^2 q_{\alpha_{\text{pred}}}(\lambda_k)^4\right]\right)^{1/2} \\
&\leq C_6\sigma^2\left(\mathbb{E}\left[\Psi_2\left(C_q\sum_{k=1}^{\infty}s_{\alpha_{\text{pred}}}(\lambda_k)^2\right)\right]\right)^{1/2} \quad [\text{by Lemma 4.3}] \\
&\leq C_6\sigma^2\left(\mathbb{E}\left[\Psi_2\left(C_q\frac{r(\alpha_{\text{pred}}, f)}{\sigma^2}\right)\right]\right)^{1/2} \quad [\text{by (12)}] \\
&\leq C_6\sigma^2\left(\Psi_2\left(2C_q\frac{r(\alpha_o, f)}{\sigma^2}\right) + C_7\right)^{1/2} \quad [\text{by Corollary 4.1}] \\
&\leq C_6(2C_q)^{1/2}\frac{\sigma\sqrt{r(\alpha_o, f)}}{S^{-1}(2C_q\frac{r(\alpha_o, f)}{\sigma^2})} + C_6(C_7)^{1/2}\sigma^2,
\end{aligned}$$

where constant C_6 depends only on $C'_q, C''_q, C_q, C_S, c_q$ and the operator T , and constant C_7 is universal.

Combining all these estimates concludes the proof. \square

5. Numerical simulations

In this section, we will investigate the behavior of the following parameter choice methods by means of a simulation study:

- (i) The oracle parameter choice $\alpha_{\text{or}} = \operatorname{argmin}_{\alpha\in\mathcal{A}}\mathbb{E}[\|\hat{f}_\alpha - f^\dagger\|_{\mathcal{X}}^2]$, which is not available in practice and evaluated here for comparison only,
- (ii) the a-posteriori parameter choice rule which is studied in this paper, given by $\alpha_{\text{pred}} = \operatorname{argmin}_{\alpha\in\mathcal{A}}\hat{r}(\alpha, Y)$ with $\hat{r}(\alpha, Y)$ as in (3),
- (iii) and the Lepskiĭ-type balancing principle originally introduced by Lepskiĭ [36], and was further developed for usage in statistical inverse problems by Bauer and Hohage [3], Mathé [44], Mathé and Pereverzev [48], and Werner and Hohage [63]. It consists in choosing

$$\alpha_{\text{LEP}} = \max\{\alpha \in \mathcal{A} \mid \|\hat{f}_{\tilde{\alpha}} - \hat{f}_\alpha\|_{\mathcal{X}} \leq 4\sigma\sqrt{\operatorname{Trace}(q_{\tilde{\alpha}}(T^*T)^2 T^*T)} \text{ for all } \tilde{\alpha} \leq \alpha, \tilde{\alpha} \in \mathcal{A}\}. \quad (24)$$

Note that the term $\sigma\sqrt{\operatorname{Trace}(q_{\tilde{\alpha}}(T^*T)^2 T^*T)}$ is in fact an upper bound for the standard deviation of $\hat{f}_{\tilde{\alpha}}$. For an explanatory derivation of this choice we refer to Mathé [44]. Unfortunately, the computation of α_{LEP} is expensive (see e.g. our simulations below).

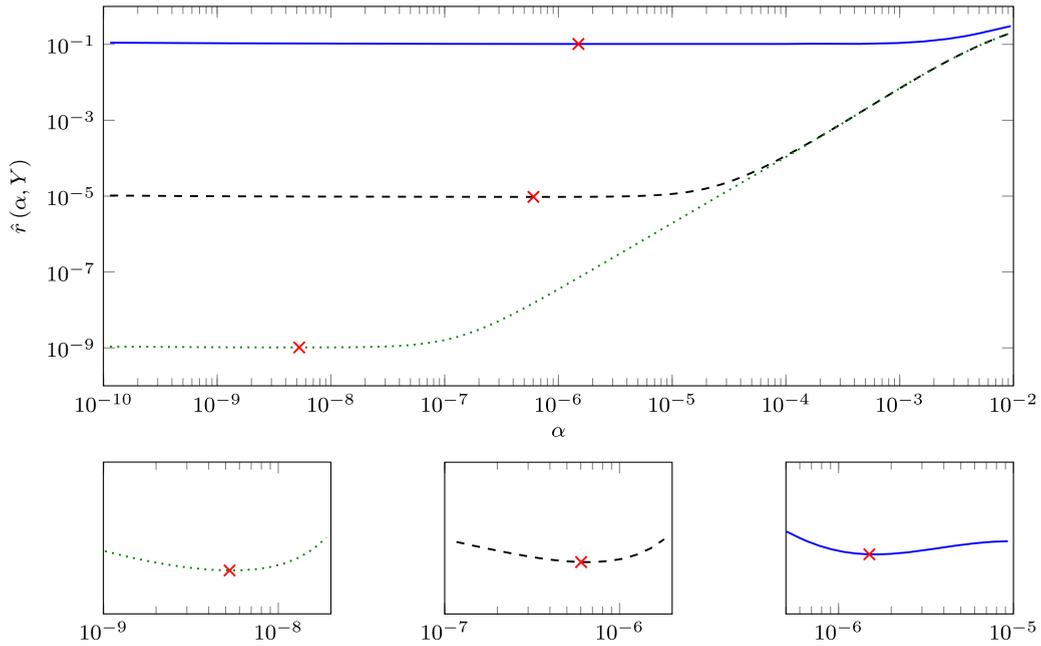


Fig. 1. The function $\alpha \mapsto \hat{r}(\alpha, Y)$ for different noise levels: $\sigma = 10^{-2}$ (—), $\sigma = 10^{-4}$ (---), $\sigma = 10^{-6}$ (⋯). We also depict zooms (not to scale) of the regions around the actual minima, which are always marked by red crosses. The operator T is as in Section 5.1, and f is as in Example 1. The chosen regularization method is Tikhonov regularization.

In all above methods, for the computational purpose, we consider a discretized version of \mathcal{A} instead by

$$\mathcal{A}_r = \{\sigma^2 \cdot r^k \mid k = 0, 1, \dots, \lfloor (\log(r))^{-1} \log(\sigma^{-2} \|T^*T\|) \rfloor\} \tag{25}$$

for some $r > 1$, i.e. it discretizes the range of possible α 's $[\sigma^2, \|T^*T\|]$ in a logarithmically equispaced way. In our simulations we use $r = 1.2$. We also tried different values of r which did not influence the results significantly. Note that it can readily be seen from the error decomposition (12) that the discrete parameter set \mathcal{A}_r is – under appropriate conditions on the filter which are satisfied by all filters in Table 1 – able to resemble the optimal behavior of a continuous parameter set $\sigma^2 \leq \alpha < \infty$ up to a constant depending on r .

Let us briefly comment on the implementation of the parameter choice rule α_{pred} . Even though the minimization is not performed over the continuum $\alpha \in \mathcal{A}$ but over a discrete set \mathcal{A}_r here, the computation of α_{pred} can be numerically challenging. In Figure 1 we depict the function $\alpha \mapsto \hat{r}(\alpha, Y)$ in an example using Tikhonov regularization, which shows that the function is relatively flat around its absolute minimum. We observed this behavior in many situations, especially if σ is not too small. However, around the minimum the function is not completely flat, and the minimum seems well-defined as visible in the zooms of Figure 1. This ensures that we will be able to find the minimum up to a discretization error determined by the value r in (25). Finally we mention that the evaluation of the trace operator in $\hat{r}(\alpha, Y)$ can be expensive, but this can be overcome by different techniques, cf. Engl et al. [22, Section 9.4] or Vogel [58, Section 7.1].

5.1. Convergence rates

At first we investigate the empirical rate of convergence in a mildly ill-posed situation. Therefore, we consider the linear integral operator $T : \mathbf{L}^2([0, 1]) \rightarrow \mathbf{L}^2([0, 1])$ defined by

$$(Tf)(x) = \int_0^1 k(x, y) f(y) dy, \quad x \in [0, 1]$$

with kernel $k(x, y) = \min\{x \cdot (1 - y), y \cdot (1 - x)\}$, $x, y \in [0, 1]$, i.e. $(Tf)'' = -f$ for all $f \in \mathbf{L}^2([0, 1])$. Obviously, the eigenvalues λ_k of T^*T satisfy $\lambda_k \sim k^{-4}$.

We discretize T by choosing equidistant points $x_1 = \frac{1}{2n}, x_2 = \frac{3}{2n}, \dots, x_n = \frac{2n-1}{2n}$ and using the composite midpoint rule

$$(Tf)(x) = \int_0^1 k(x, y) f(y) dy \approx \frac{1}{n} \sum_{i=1}^n k(x, x_i) f(x_i)$$

on the grid points $x = x_j$, $1 \leq j \leq n$. To avoid an inverse crime, the exact data Tf is always calculated analytically. The discretization parameter n is set to 1024.

We consider two different scenarios varying in the smoothness of the unknown solution f :

Example 1. As the first example, we consider the continuous function

$$f(x) = \begin{cases} x & \text{if } 0 \leq x \leq \frac{1}{2}, \\ 1 - x & \text{if } \frac{1}{2} \leq x \leq 1. \end{cases}$$

It can readily be seen by straightforward computations that the Fourier coefficients f_k of f are given by

$$f_k = \frac{(-1)^k - 1}{4\pi^3 k^2}.$$

Consequently $f \in \mathcal{S}_{3-\varepsilon}$ and we obtain $\mathcal{O}(\sigma^{\frac{3}{4}-\varepsilon})$ as rate of convergence for any $\varepsilon > 0$, see Corollary 3.4.

Example 2. In the second example we choose

$$f(x) = \begin{cases} 1 & \text{if } \frac{1}{4} \leq x \leq \frac{3}{4}, \\ 0 & \text{else.} \end{cases}$$

As this function can be written as the derivative of functions as in the first example, it is clear that $f \in H^{\frac{1}{2}-\varepsilon}([0, 1])$ for any $\varepsilon > 0$. This is also evident by the fact that the Fourier coefficients f_k of f are given by

$$f_k = \frac{(-1)^k \sin(\frac{\pi k}{2})}{2\pi^2 k}.$$

Consequently, $f \in \mathcal{S}_{1-\varepsilon}$ and we obtain $\mathcal{O}(\sigma^{\frac{1}{3}-\varepsilon})$ as rate of convergence for any $\varepsilon > 0$, see Corollary 3.4.

Remark 11. In the present setting, it follows from results by Hohage and Weidling [30] that one can obtain a rate of convergence $\mathcal{O}(\sigma^p)$ for a function f if and only if $f \in B_{2,\infty}^{\frac{5p}{4-2p}}$ the L^2 -based Besov-space $B_{2,\infty}^s$ with smoothness index s and fine index ∞ . Consequently, in the above mentioned Examples 1 and 2, one finds that the minimax rates of convergence are $\mathcal{O}(\sigma^{\frac{3}{4}})$ and $\mathcal{O}(\sigma^{\frac{1}{3}})$ respectively.

In Figure 2 we plot several empirical risks against the noise level $\sigma \in \{2^{-15}, \dots, 2^{-25}\}$. The optimal rate of convergence taking into account Remark 11 is also indicated. We consider spectral cut-off (cf. Figure 2(a)), Tikhonov regularization (cf. Figure 2(b)), and Showalter regularization (cf. Figure 2(c)). Using Monte Carlo simulations with 10^4 experiments per noise level we compute empirical versions of the oracle risk $R_{\text{or}}(\sigma) := \mathbb{E}[\|\hat{f}_{\alpha_{\text{or}}} - f^\dagger\|_2^2]$, the prediction risk $R_{\text{pred}}(\sigma) := \mathbb{E}[\|\hat{f}_{\alpha_{\text{pred}}} - f^\dagger\|_2^2]$, and the Lepskiï risk $R_{\text{LEP}}(\sigma) := \mathbb{E}[\|\hat{f}_{\alpha_{\text{LEP}}} - f^\dagger\|_2^2]$.

In all plots we find a good agreement of our theoretical predictions and the empirical results. Compared with the Lepskiï-type balancing principle, it seems that α_{pred} performs order-optimal with a slightly smaller constant. The loss of a log-factor by using α_{LEP} cannot be visible in such a small simulation study. We furthermore estimated the empirical rates from the simulations depicted in Figure 2 and compared them by means of statistical testing with the minimax rate of convergence. In all cases, the hypothesis test described in Appendix B accepts the hypothesis that the empirical prediction risk rate is at least the minimax rate with significance level 10%. In view of Remark 11, a faster rate of convergence is impossible. From this point of view, our simulations strongly support the theory.

5.2. Efficiency simulations

Besides the convergence rate simulations above we also want to numerically infer on the constant in the oracle inequality which will be done by efficiency simulations. Therefore (inspired by [4,15]) we consider the following setup. The forward operator is a 300×300 diagonal matrix with singular values $\lambda(k) = k^{-a}$ with a fixed parameter $a > 0$. Then we repeat the following experiment 10^4 times: Given a parameter ν we generate a random ground truth $f \in \mathbb{R}^{300}$ by $f(k) = \pm k^{-\nu} \cdot (1 +$

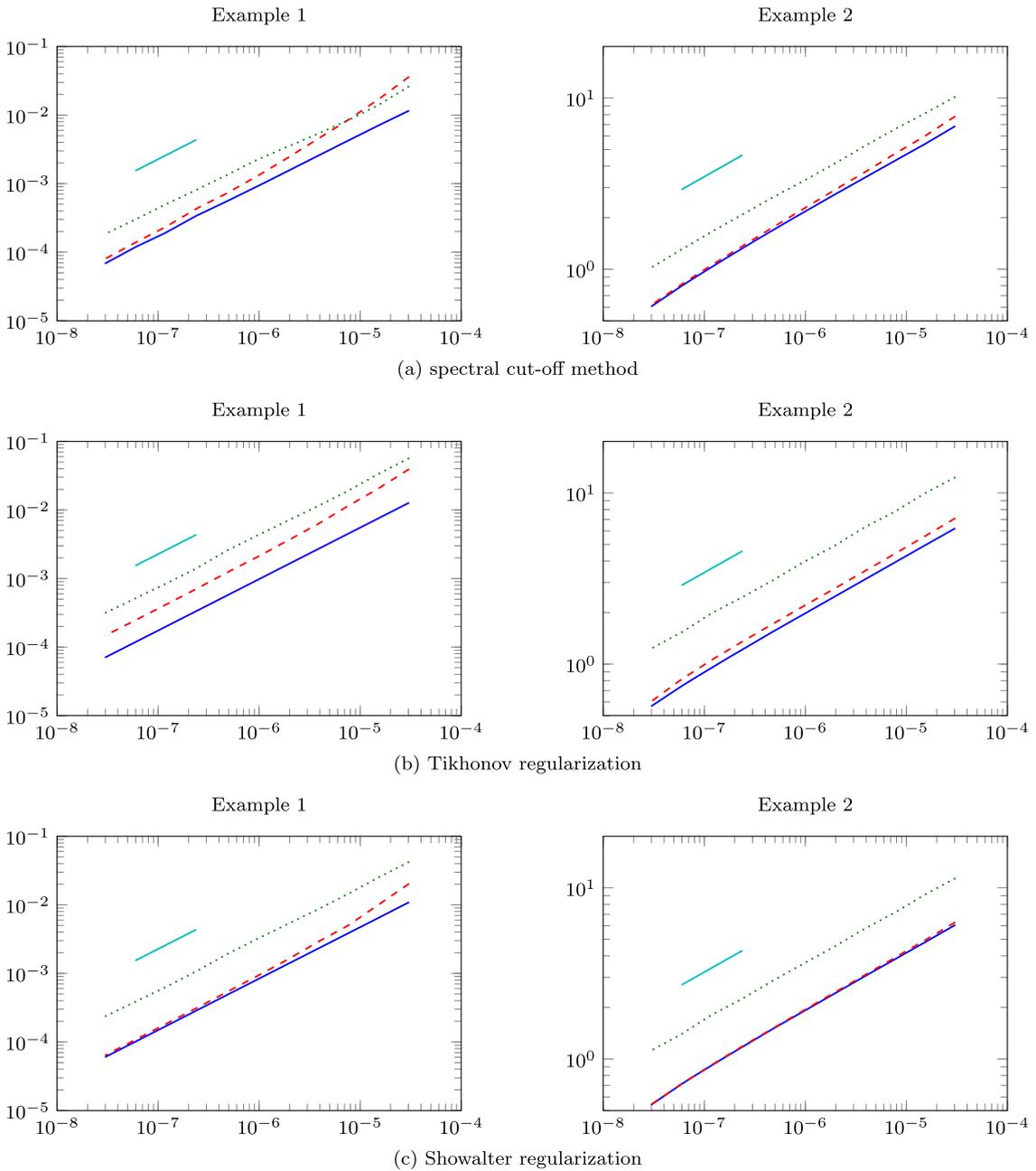


Fig. 2. Simulation results for various regularization methods: the oracle risk R_{or} (—), the prediction risk R_{pred} (- - -), the Lepski risk R_{LEP} (⋯), and the optimal rates of convergence $\sigma^{3/4}$ and $\sigma^{1/3}$ respectively (—) as functions of σ for the two considered examples.

$\mathcal{N}(0, 0.1^2)$) where the sign is independent and uniformly distributed for each component. From this ground truth, data is generated according to $Y(k) = \lambda(k) \cdot f(k) + \mathcal{N}(0, \sigma^2)$ where the noise is again independent in each component. Based on the data we compute empirical versions of the oracle risk $R_{\text{or}}(\sigma)$, the prediction risk $R_{\text{pred}}(\sigma)$, and the Lepski risk $R_{\text{LEP}}(\sigma)$ for Tikhonov regularization. In Figure 3 we depict the fractions of the oracle risk with the different a-posteriori risks for various parameters ν and a to compare the average behavior of these parameter choice methods.

In conclusion we empirically find that both choices α_{pred} and α_{LEP} seem to satisfy an oracle inequality. Comparing the performance of α_{pred} and α_{LEP} it seems that α_{LEP} behaves worse for small values of σ , which is in good agreement with Figure 2. Furthermore, the computational effort for α_{pred} is significantly smaller: in our efficiency simulations around 90% of the computation time were spent for computing α_{LEP} in (24).

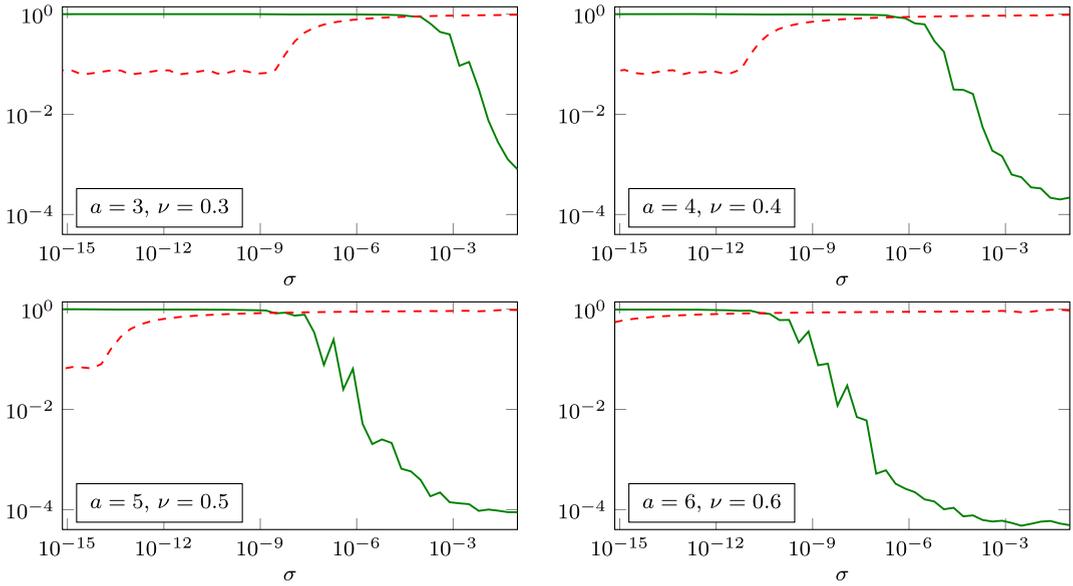


Fig. 3. Efficiency simulations for Tikhonov regularization with different smoothness parameters a and ν : $R_{\text{or}}/R_{\text{pred}}$ (—), $R_{\text{or}}/R_{\text{LEP}}$ (- - -).

6. Conclusion and outlook

In this study we have analyzed a parameter choice method for filter-based regularization methods applied to linear statistical inverse problems. Therefore we have proven an oracle inequality, which generalizes the one from Chernousova and Golubev [15] to general ordered filters satisfying weak assumptions (cf. Definition 1 and Assumption 3). From this oracle inequality we derived convergence rates of the investigated parameter choice, which are actually order optimal in a wide range of cases.

We point out that our techniques do not seem to be limited to the specific choice of α investigated here. Quite the contrary, we provide a general strategy to prove an oracle inequality, which might be used for other choices as well. If one would consider a different parameter choice rule, then an oracle inequality can be carried out the same way as in this study provided the following ingredients are available:

- general moment bounds for the prediction risk as in Corollary 4.1 (in our case based on the exponential bounds proven by Kneip [35]),
- a deterministic optimality result as in Lemma 4.2,
- estimates for the behavior of the regularization algorithm as in Lemma 4.3.

Note that the latter two assumptions do not rely on the parameter choice rule at all but only on the interplay of the operator, the regularization method, and the source condition. Consequently, whenever the general moments can be bounded, the analysis can basically be carried over from standard results, see e.g. Bellec and Tsybakov [5] for a useful deviation inequality for regularization methods with convex penalties.

Even though we have always assume that the noise level σ is known, the generalization to unknown σ is straightforward. For the choice of parameter α_{pred} , we simply replace σ by a proper estimator $\hat{\sigma}$ in (3) and (13). The only affected part in our argumentation is the Kneip's deviation bound in Theorem 2.1, which still holds if we further assume the smoothness of Tf (this is usually the case due to the blessing of ill-posedness). More precisely, one could consider estimators of the form $\hat{\sigma}^2 := \langle Y, \Lambda_\sigma Y \rangle_{\mathcal{Y}^* \times \mathcal{Y}}$ for some linear operator Λ_σ such that $\mathbb{E}[\langle \xi, \Lambda_\sigma \xi \rangle_{\mathcal{Y}^* \times \mathcal{Y}}] = 1$ and $\text{Trace}(\Lambda_\sigma^* \Lambda_\sigma) \leq C < \infty$. In this case, under additional smoothness assumption that $|\langle Tf, \Lambda_\sigma Tf \rangle_{\mathcal{Y}}| \leq \tilde{C} \sigma^2$, the assertion of Theorem 2.1 still holds, with constants C'_ξ, C''_ξ there depending only on C and \tilde{C} , see [28] for a possible choice of Λ_σ , and Section 6 in [35] for further details.

Another possible generalization concerns the errors in (1). If ξ is such that the ξ_k 's in (5) are independent sub-Gaussian errors, then there are two crucial parts of the proofs which have to be generalized: Theorem 2.1 and Lemma 4.4. In fact it turns out that both also hold for independent sub-Gaussian errors (see [27,35]), so the whole analytical methodology remains valid in such a case as well.

The general analytical strategy advocated in this paper, of course, has its own limitations, as the resulting oracle inequality might turn out to be inadequate or even trivial in certain cases (see Section 3.3.2 for instance). For exponentially

ill-posed problems, we expect that the parameter choice rule under investigation has to be modified suitably, as examined in the seminal papers [13,26]. Future questions include generalizations to nonlinear problems and noise models with heavier tails.

Appendix A: Properties of α_{pred}

We first show that almost surely the infimum of $\hat{r}(\alpha, Y)$ in (13) over α in \mathcal{A} is attainable, and such a minimizer is unique. The existence of minimizers follow immediately from the continuous dependence of $q_\alpha(\lambda)$ on α and the closedness of \mathcal{A} . For the uniqueness, we focus on the case that $Y_k \neq 0$ for every $k \in \mathbb{N}$, which holds with probability 1. Define $\tilde{r} : \ell^\infty \rightarrow \mathbb{R}$ as

$$\tilde{r}(x) = \sum_{k=1}^{\infty} \lambda_k^2 Y_k^2 x_k^2 - 2 \sum_{k=1}^{\infty} \lambda_k Y_k^2 x_k + 2\sigma^2 \sum_{k=1}^{\infty} \lambda_k x_k \quad \text{for every } x = \{x_k\}_{k \in \mathbb{N}} \in \ell^\infty.$$

It is easy to see that $\tilde{r}(\cdot)$ is strictly convex. Note that $\hat{r}(\alpha, Y) = \tilde{r}(x)$ with $x = \{q_\alpha(\lambda_k)\}_{k \in \mathbb{N}}$. This, together with the fact that q_α is strictly increasing over α , implies the uniqueness of $\operatorname{argmin}_{\alpha \in \mathcal{A}} \hat{r}(\alpha, Y)$. Thus, α_{pred} is well-defined.

Next we consider the measurability of α_{pred} . Due to its uniqueness, we have for any $x \in \mathbb{R}$

$$\{\alpha_{\text{pred}} < x\} = \left\{ \min_{\alpha \in \mathcal{A}} r(\alpha, Y) < \min_{\alpha \in \mathcal{A}, \alpha \geq x} r(\alpha, Y) \right\} = \bigcup_{z \in \mathbb{Q}} \left(\left\{ \min_{\alpha \in \mathcal{A}} r(\alpha, Y) < z \right\} \cap \left\{ \min_{\alpha \in \mathcal{A}, \alpha \geq x} r(\alpha, Y) > z \right\} \right).$$

By the continuity of q_α with respect to α , it holds that $\{\min_{\alpha \in \mathcal{A}} r(\alpha, Y) < z\}$ and $\{\min_{\alpha \in \mathcal{A}, \alpha \geq x} r(\alpha, Y) > z\}$ are measurable. Then $\{\alpha_{\text{pred}} < x\}$ is measurable, and thus α_{pred} is measurable.

Appendix B: Hypothesis testing for rates of convergence

In our simulations, we fix a test function f , select a sequence of noise levels $\{\sigma_i : i = 1, \dots, n\}$, and for each σ_i we compute estimators $\hat{f}_{\sigma_i, j}$ of f from independent realizations of Y for every $j = 1, \dots, m$. This gives rise to an empirical estimate $\bar{e}_i := \sum_{j=1}^m e_{i,j} / m$ of the risk $\mathbb{E}[\|\hat{f}_{\sigma_i} - f\|_{\mathcal{X}}^2]$ with $e_{i,j} := \|\hat{f}_{\sigma_i, j} - f\|_{\mathcal{X}}^2$. To estimate the convergence order ϑ in $\mathbb{E}[\|\hat{f}_{\sigma_i} - f\|_{\mathcal{X}}^2] \approx C\sigma_i^\vartheta$, we assume the model

$$\log \bar{e}_i = \vartheta \log \sigma_i + \varrho + \varepsilon_i \quad \text{with } \varepsilon_i \sim \mathcal{N}(0, \delta_i^2) \text{ independently, } i = 1, \dots, n. \quad (26)$$

Here ϑ , and ϱ are unknown, and we assume for the moment that standard deviations δ_i of perturbation are known in advance. Note that it is not possible to achieve faster convergence rates than the optimal one. In order to investigate the discrepancy between the convergence rate of \hat{f}_σ and the optimal one, it is sufficient to test whether it is no slower than the optimal rate or not. To be precise, we consider the test

$$H_0 : \vartheta \geq \vartheta_o \quad \text{against} \quad H_1 : \vartheta < \vartheta_o,$$

where ϑ_o is the optimal order of convergence for test function f .

From linear model theory (e.g. [50]), a classical testing statistics (based on the MLE estimator of ϑ_o) for the above test is

$$\begin{aligned} \mathbb{T} &:= (\hat{\vartheta} - \vartheta_o) \left(\frac{(\sum_{i=1}^n \delta_i^{-2})(\sum_{i=1}^n \delta_i^{-2} \log^2 \sigma_i) - (\sum_{i=1}^n \delta_i^{-2} \log \sigma_i)^2}{\sum_{i=1}^n \delta_i^{-2}} \right)^{1/2} \\ \text{with } \hat{\vartheta} &= \frac{(\sum_{i=1}^n \delta_i^{-2})(\sum_{i=1}^n \delta_i^{-2} \log \sigma_i \log \bar{e}_i) - (\sum_{i=1}^n \delta_i^{-2} \log \sigma_i)(\sum_{i=1}^n \delta_i^{-2} \log \bar{e}_i)}{(\sum_{i=1}^n \delta_i^{-2})(\sum_{i=1}^n \delta_i^{-2} \log^2 \sigma_i) - (\sum_{i=1}^n \delta_i^{-2} \log \sigma_i)^2}. \end{aligned} \quad (27)$$

The corresponding rejection region of significance level $\alpha \in (0, 1)$ is $R_\alpha := \{\mathbb{T} < z_{1-\alpha}\}$, and the corresponding p -value is $\Phi(\mathbb{T})$, where $z_{1-\alpha}$ and Φ are the $(1-\alpha)$ quantile and the distribution function of the standard normal distribution, respectively. In reality, the standard deviations δ_i are unknown, but can be easily estimated from the sample variance of $\{e_{i,j}\}_{j=1}^m$ by means of delta methods. More precisely, the central limit theorem implies $\sqrt{m}(\bar{e}_i - \mathbb{E}[e_{i,j}]) \xrightarrow{D} \mathcal{N}(0, \operatorname{Var}[e_{i,j}])$, and via delta methods we obtain

$$\sqrt{m}(\log \bar{e}_i - \log \mathbb{E}[e_{i,j}]) \xrightarrow{D} \mathcal{N}(0, \mathbb{E}[e_{i,j}]^{-2} \operatorname{Var}[e_{i,j}]).$$

Then $\text{Var}[\log \bar{e}_i] \approx m^{-1} \mathbb{E}[e_{i,j}]^{-2} \text{Var}[e_{i,j}]$. Based on such an approximation, we derive an estimator of δ_i as

$$\hat{\delta}_i := \frac{1}{\sqrt{m} |\bar{e}_i|} \left(\sum_{j=1}^m (e_{i,j} - \bar{e}_i)^2 \right)^{1/2}.$$

The final procedure is given by (27) with δ_i replaced by $\hat{\delta}_i$, which is exactly the testing procedure used in Section 5. We note that one can justify the model (26) and the estimation of δ_i by using a large m .

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