Tikhonov regularization in Hilbert scales for nonlinear statistical inverse problems

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Contents

Chapter 1

Introduction

'Solution of an inverse problem entails determining unknown causes based on observation of their effects. This is in contrast to the corresponding direct problem, whose solution involves finding effects based on a complete description of their causes.' This is probably the best statement about what inverse problems mean, description due to O.M. Alifanov. These type of problems appear in many fields e.g. physics, biology, medicine, chemistry and geology. Inverse scattering, which tries to reconstruct an obstacle or an inhomogeneity from scattered waves (see e.g. [CK98]), deblurring and denoising in image processing (see e.g. [BB98]), parameter identification in diffusion processes, groundwater hydrology or biology (see e.g. [BK89]) are just some examples of inverse problems that we need to solve in applications.

From a mathematical point of view the aim of inverse problems is to approximately invert a forward operator, which models usually a well understood problem. We consider the inverse problem to estimate a quantity $a^\dagger$ in a separable Hilbert space $\mathcal{X}$, which is not directly observable. We only have access to a vector $u^\dagger$ in another Hilbert space $\mathcal{Y}$, and the relation between $a^\dagger$ (the 'exact solution') and $u^\dagger$ (the 'exact data') is described by some possibly nonlinear operator $F : D(F) \subset \mathcal{X} \to \mathcal{Y}$

$$F(a^\dagger) = u^\dagger. \tag{1.1}$$

We are interested in the case when the problem (1.1) is ill-posed. This notion is due to Hadamard, who stated that a well-posed problem has a unique solution depending continuously on the data. At the beginning of the 20-th century an appropriate model for a physical phenomenon was considered a well-posed one, the other situation was named 'ill-posed'. A milestone in the development of the regularization theory, which deals with the ill-posedness of the problems, was the early work of Tikhonov. Subsequently, the subject was often studied by mathematicians (see e.g. [EHN96, Kir96]). First, linear inverse problems, that correspond to a linear operator F, were thoroughly investigated. In the last decade there was a growing interest in nonlinear inverse problems in a deterministic setting (see [EHN96, Kir96]). In this thesis we assume that the operator F

is nonlinear, one-to-one, but the inverse of F is not assumed to be continuous (the solution of the equation does not depend continuously on the data). The instability of the problem is important because the data usually contain noise, due to the measurement process.
We consider that we have at our disposal the noisy data Y

$$Y = F(a^\dagger) + \delta\xi + \sigma\epsilon \tag{1.2}$$

which contain additive deterministic and stochastic noise with known noise levels δ and σ respectively. Here $\xi \in \mathcal{Y}$, $\|\xi\|_\mathcal{Y} = 1$ denotes the normalized deterministic error, and ϵ denotes a normalized noise process in $\mathcal{Y}$, which will be defined in Chapter 2. In that chapter we will also motivate the choice of this general noise model and its relation to other well-known stochastic models. In the following we always assume that the covariance operator of ϵ is known (e.g. the identity for the white noise), which is reasonable in many cases.
We construct and analyse in this thesis an estimator $\widehat{a}$ of $a^\dagger$ starting from the noisy data Y. To cope with the discontinuity of the inverse of F, a regularization scheme is usually chosen, i.e. a parametrized family R_α of continuous operators, pointwise converging towards F^{-1}. This family, together with a rule for choosing the regularization parameter $\alpha(\delta, \sigma, Y)$, is a regularization method if the worst case expected error

$$\Delta_R(\delta, \sigma, a^\dagger, F) = \sup\left\{ (\mathbf{E}\|R_{\alpha(\delta,\sigma,Y)}(Y) - a^\dagger\|^2)^{\frac{1}{2}} : Y = F(a^\dagger) + \delta\xi + \sigma\epsilon, \|\xi\|_\mathcal{Y} \le 1 \right\}$$

converges to zero when $\delta, \sigma \to 0$ for all $a^\dagger \in D(F)$. We distinguish between two different types of strategies for the choice of the regularization parameter: a-priori (that depend only on the noise levels) and a-posteriori (that depend both on the noise levels and the data Y).
In a deterministic setting, one possible method to solve the nonlinear ill-posed problem (1.1) is Tikhonov regularization. This consists in approximating the solution of the problem (1.1) by the solution $\widehat{a}$ of the minimization problem

$$\widehat{a} = \operatorname{argmin}_{a \in D(F)} \|F(a) - Y\|^2_\mathcal{Y} + \alpha\|a - a_0\|^2_\mathcal{X}$$

where $\alpha > 0$ is a regularization parameter and $a_0 \in \mathcal{X}$ is an initial guess. Convergence analysis of this method for deterministic nonlinear inverse problems for a-priori and a-posteriori choices of the regularization parameter is due to Engl, Kunisch and Neubauer (see [EKN89, Neu89]). A review of these results is presented in section 2.4.
Another possible technique to solve the nonlinear inverse problem (1.1) is Newton's method. We consider the linearized equation

$$F'(a_k)h_k = Y - F(a_k) \tag{1.3}$$

in which the update $a_{k+1} - a_k = h_k$ is to be computed. Since this linear problem usually inherits the ill-posedness of the nonlinear problem, a regularization method is required.
Levenberg-Marquardt method is an iterative method which is equivalent to Tikhonov regularization applied to the linearized problem for a given current approximation a_k of $a^\dagger$ (see e.g. [Han97]). The update h_k is the solution of the minimization problem

$$h_k = \operatorname{argmin}_{h\in\mathcal{X}} \|Y - F(a_k) - F'(a_k)h\|^2_{\mathcal{Y}} + \alpha_k \|h\|^2_{\mathcal{X}}.$$

Convergence analysis and rates of convergence results for a-posteriori choice of the regularization parameter (by discrepancy principle) and for a-priori choice of the regularization parameter are given in [Han97, Rie99].
Stability can be further increased by regularizing around some fixed element a_0, i.e. by applying Tikhonov regularization with initial guess $a_k - a_0$ to the Newton equation (1.3), leading to the minimization problem

$$\min_{h\in\mathcal{X}} \|Y - F(a_k) - F'(a_k)h\|^2_{\mathcal{Y}} + \alpha_k \|h + a_k - a_0\|^2_{\mathcal{X}} \tag{1.4a}$$

or equivalently

$$(\alpha_k I + F'(a_k)^* F'(a_k))h_k = F'(a_k)^*(Y - F(a_k)) + \alpha_k(a_0 - a_k). \tag{1.4b}$$

This yields the iteratively regularized Gauss-Newton method which was suggested by Bakushinskii (see [Bak92]). Convergence analysis for regularized Newton methods with a-priori and a-posteriori (with discrepancy principle) choice of the regularization parameter was given in [BNS97, Kal97, Hoh99].
The regularized Newton methods have the advantage of an explicit iteration formula (e.g. (1.4b)), but general convergence results are always local ones (see e.g. [Kal97]). On the other hand, global convergence results for nonlinear Tikhonov regularization were proved, but this method requires solving a global minimization problem, which might have several (even local) minima. More restrictive assumptions are required to ensure uniqueness of a global minimum. Iterative algorithms that numerically compute this minimum are developed ([Ram03, LPR07, RT05]). Ramlau proposed in this case a combination between Tikhonov regularization and a gradient method (TIGRA). In our thesis we construct the estimator $\widehat{a}$ with the help of Tikhonov regularization.
Since it is known that the error $\Delta_R(\delta, \sigma, a^\dagger, F)$ may tend to 0 arbitrarily slowly as $\delta, \sigma \to 0$ (see [EHN96]), we impose smoothness condition on $a^\dagger$, known as source conditions in deterministic setting. The source sets considered correspond to so called 'Hölder source conditions', i.e.

$$X_{\mu,\rho} = \{a \in \mathcal{X} : a = (B^*B)^\mu w, \|w\| \le \rho\}$$

where B is a smoothing operator. Usually, the operator B coincides with F if F is linear or with $F'(a^\dagger)$ in the nonlinear case. Although the abstract source conditions appear naturally in a functional analytic setting and they are not only sufficient but even almost necessary for certain rates of convergence, they are often difficult to interpret. Another possibility to define appropriate smoothness conditions is with the help of the Hilbert scales. Hilbert scales are defined as a family of Hilbert spaces $\mathcal{X}_s$ with the inner products $\langle u, v\rangle_s = \langle L^s u, L^s v\rangle_{\mathcal{X}}$, where L is an unbounded, densely defined, self-adjoint, strictly positive operator. Typically L is a differential operator, and the spaces $\mathcal{X}_s$ are closed subsets of Sobolev spaces. Therefore this leads to very natural and explicit smoothness assumptions. However, the conditions relating the operator F and the Hilbert scale required by convergence theorems are often not satisfied for the standard Hilbert scales. This makes it necessary to define problem dependant Hilbert scales, which is an elaborate task. In Chapter 3 we review some some tools for constructing self-adjoint operators and Hilbert scales.
The maximal risk of a regularization method R on a smoothness class $\tilde{\mathcal{X}} \subseteq \mathcal{X}$ is defined as

$$\Delta_R(\delta, \sigma, \tilde{\mathcal{X}}, F) := \sup_{a^\dagger \in \tilde{\mathcal{X}}} \Delta_R(\delta, \sigma, a^\dagger, F).$$

The best possible lower bound on the maximal risk is the so-called minimax risk

$$\Delta(\delta, \sigma, \tilde{\mathcal{X}}, F) = \inf_R \Delta_R(\delta, \sigma, \tilde{\mathcal{X}}, F).$$

Starting with the seminal paper of Pinsker [Pin80] sharp lower bounds for the minimax risk have been derived for linear operator F (see also [Tsy04, Don94]). We study not only the rates of convergence but also the optimality with respect to the linear minimax rates of our estimator $\widehat{a}$, constructed with the help of Tikhonov regularization in Hilbert scales. Whereas there exists a considerable literature on linear statistical inverse problems, only a few results on nonlinear statistical inverse problems have been obtained until now. A first method for nonlinear inverse problems in the statistical setting, inspired by Tikhonov regularization and named Method of Regularization, was studied by O'Sullivan, Lukas and Wahba (see [O'S90, Luk06, Wah90]). They consider the problem (1.1) in a discretized setting, with the functionals $F_i : D(F) \subset \mathcal{X} \to \mathbf{R} \quad i = 1, \dots, n$ which are typically of form $F_i(a) = (F(a))(X_i)$ if $\mathcal{Y}$ is an L^2-space and data $Y_i = F_i(a) + \sigma\epsilon_i$. Then $a^\dagger$ is approximated by the solution of the minimization problem

$$\widehat{a} = \operatorname{argmin}_{a \in D(F)} \frac{1}{n} \sum_{i=1}^{n} |F_i(a) - Y_i|^2 + \alpha \|a - a_0\|^2_{\mathcal{X}}.$$

The straightforward generalization to the infinite-dimensional noise model (1.2) is

$$\widehat{a} := \operatorname{argmin}_{a \in D(F)} \left(\|F(a) - Y\|^2_{\mathcal{Y}} + \alpha \|a - a_0\|^2_{\mathcal{X}} \right).$$

However, in the most important case that ϵ is white noise, $\|F(a)-Y\|$ is infinite with probability 1 for all $a \in D(F)$, so $\widehat{a}$ is not well-defined. Therefore, as in [BHM04] we consider a two-step estimator, which in our case looks as follows:

- The first step consists in determining an estimator $\widehat{u}$ of u from the data Y. This is a nonparametric regression problem which has been studied intensively in the statistical literature (see [Tsy04] and references therein). We assume that the error estimate

$$\sqrt{\mathbf{E}\|\widehat{u}-u^\dagger\|_{\mathcal{Y}}^2} \leq \beta. \tag{1.5}$$

  holds true. β will play the role of the noise level in the next step. Even for $\delta = 0$, $\widehat{u}$ has to be biased in general, i.e. $\mathbf{E}\widehat{u} \neq u^\dagger$.

- In the second step we construct the estimator $\widehat{a}$ as the solution of the Tikhonov minimization problem

$$\widehat{a} := \operatorname{argmin}_{a\in D(F)\cap(a_0+\mathcal{X}_s)} \left(\|F(a)-\widehat{u}\|_{\mathcal{Y}}^2 + \alpha\|a-a_0\|_s^2\right).$$

Chapter 4 is devoted to the convergence analysis of the estimator $\widehat{a}$. Consistency, i.e.$\lim_{\beta\to 0}\mathbf{E}\|\widehat{a}-a^\dagger\|_{\mathcal{X}}^2 = 0$ has already been shown in [BHM04]. We derive a convergence rate estimate in terms of β if $a^\dagger - a_0 \in \mathcal{X}_q$ and q belongs to a certain interval. A similar result for deterministic noise has been obtained by Neubauer [Neu92], but it turns out that more restrictive assumptions on F are required for stochastic noise. A special convergence rate estimate for stochastic noise with a Hölder smoothness condition of index $\mu = \frac{1}{2}$ was previously obtained in [BHM04]. We study the general optimality of the method with respect to the stochastic noise level σ, and we conclude that the minimax rates are attained in the case of linear operators. We also discuss optimality of our method for nonlinear operators.
Typically, a-priori rules require a-priori knowledge of the smoothness of the solution to obtain optimal rates of convergence whereas certain a-posteriori rules do not need such a-priori knowledge. In Chapter 5 we present a short description and interpretation of Lepskii's balancing principle. Afterwards, we obtain order-optimal rates of convergence for this a-posteriori choice of the regularization parameter in the deterministic setting and almost-optimal in the stochastic setting.
The next chapter is dedicated to applications. We consider two parameter identification problems for elliptic differential equations and a Hammerstein integral equation, and we show that the rates of convergence proved before for the estimator $\widehat{a}$ are valid for these examples, since the assumptions of the theorems hold for these problems. This involves the construction of appropriate Hilbert scales for each example.
In the last chapter we illustrate the rates of convergence proved in Chapter 4 for

the first parameter identification problem presented in Chapter 6. We discuss local polynomial estimators, and we construct the estimator $\widehat{u}$ in this way. Then we compute $\widehat{a}$ numerically by the Levenberg-Marquardt algorithm. It turns out that the rates exhibited by our numerical estimator match those predicted by the convergence theorems.

Chapter 2

Regularization methods in statistical inverse problems

Inverse problems are formulated differently and raise distinct questions for a statistician and an applied mathematician. In this chapter we present these points of view in one framework, underlying the similarities and distinctions between the two standpoints. In the first section we state the inverse problem in a general noise model, which allows both deterministic as stochastic noise and which is the framework necessary to obtain our results. Then we review the optimality criteria and conditions for a class of methods needed to give 'reasonable' answers in unstable situations ('regularization methods') which are usually used in deterministic setting. Afterwards, the analogous presentation of some criteria measuring the quality of a statistical estimator is the object of our study. The last two sections contain a short survey of optimality results for Tikhononv regularization for nonlinear inverse problems in deterministic and statistical framework.

2.1 Noise model

In practice, we want to draw conclusions about a phenomenon having at our disposal noisy data. Moreover, the output is observed only in a discretized or binned form. It is also natural to assume that we are given an independent, identically distributed sample $(Y_1, \ldots, Y_n)$ of random elements on a probability space $(\Omega, \mathcal{K}, \mathbf{P})$ which are in some sense directly related to the exact data $u^\dagger$. For example, in the case of the indirect regression problem the relation between the data $(Y_i)_{i=1\ldots n}$ and the value to estimate $a^\dagger$ consists of

$$Y_i = \left(F(a^\dagger)\right)(X_i) + \varepsilon_i, \qquad i = 1, .., n \tag{2.1}$$

where $F : \mathcal{X} \to \mathcal{Y}$, $F(a^\dagger) = u^\dagger$ is the operator introduced in (1.1). If $u^\dagger$ describes the solution to a differential equation in a domain $\Omega \subset \mathbf{R}^d$, a natural choice for the space $\mathcal{Y}$ is $L^2(\Omega)$. For theoretical purposes it is often convenient to work with a white noise model. In the case that $F = I$ and we observe a trajectory $\{Y_t^n(t), t \in [0,1]\}$ of the continuous Gaussian process Y

$$dY_t^n = u^\dagger(t)\,dt + \frac{\sigma(t)}{\sqrt{n}}\,d\varepsilon_t + \delta_n(t)\,dt \tag{2.2}$$

where ε_t is Brownian motion and δ_n is a small 'drift' term, it was proved that asymptotical results in the continuous Gaussian white noise model are similar to asymptotical theory in the discrete model (2.1) as $n \to \infty$ (see e.g. [Nus96, BL96]).
That's why we consider the noise model

$$Y = u^\dagger + \delta\xi + \sigma\epsilon \tag{2.3}$$

where $\xi \in \mathcal{Y}$, $\|\xi\| \leq 1$ is the normalized deterministic error, ϵ is a normalized Hilbert space process that will be defined below and τ, δ are the corresponding deterministic and stochastic noise levels. This general noise model is inspired by [MP01] and was investigated in [BHMR07]. We are going to study separately the case of deterministic, respectively stochastic error with the corresponding noise levels.
In the general noise model the stochastic error is a **Hilbert-space process** $\epsilon \in L(\mathcal{Y}, L^2(\Omega, \mathcal{K}, \mathbf{P}))$, this means a continuous, linear operator defined between $\mathcal{Y}$ and $L^2(\Omega, \mathcal{K}, \mathbf{P})$. The relation between this general noise model and the discrete one (2.1) was studied in [BHMR07], where it was proved that the first is a generalization of the latter, since it allows not only uniform but also general random design.
The **covariance operator** of a Hilbert-space process ϵ $\mathbf{cov}_\epsilon : \mathcal{Y} \to \mathcal{Y}$ is the bounded, linear operator, defined implicitly by

$$\langle \mathbf{cov}_\epsilon \varphi_1, \varphi_2 \rangle = \mathbf{cov}(\langle \epsilon, \varphi_1 \rangle, \langle \epsilon, \varphi_2 \rangle), \varphi_1, \varphi_2 \in \mathcal{Y}.$$

A **white noise process** is a Hilbert-space process such that $\mathbf{cov}_\epsilon = I$ and for all $\varphi \in \mathcal{Y}$, $\mathbf{E}\,\langle \epsilon, \varphi \rangle_{\mathcal{Y}} = 0$. If, for a white noise process ϵ, $\langle \epsilon, \varphi \rangle_{\mathcal{Y}}$ is a Gaussian random variable for all $\varphi \in \mathcal{Y}$, we call this a **Gaussian white noise process**.
Another idea would be define the stochastic error as a **Hilbert-space valued random variable** Σ with second order moments, i.e.

$$\Sigma \in \mathcal{F} = \left\{ \tilde{\Sigma} : \Omega \to \mathcal{Y},\ \text{measurable}\ , \mathbf{E}\|\tilde{\Sigma}\|_{\mathcal{Y}}^2 < \infty \right\}$$

where $(\Omega, \mathcal{K}, \mathbf{P})$ is the underlying space of probability.
Any Hilbert-space valued random variable with finite second moment can be identified with a Hilbert-space process with the help of the mapping

$$\begin{aligned} &\mathcal{F} \to L(\mathcal{Y}, L^2(\Omega, \mathcal{K}, \mathbf{P})), \\ &\Sigma \mapsto \varepsilon, \varepsilon(\varphi) := \langle \Sigma, \varphi \rangle_{\mathcal{Y}}\,. \end{aligned}$$

This mapping is well-defined because

$$\begin{aligned}\mathbf{E}\left(|\left\langle \Sigma,\varphi\right\rangle_{\mathcal{Y}}|^2\right) &\le \mathbf{E}(\|\Sigma\|_{\mathcal{Y}}^2\|\varphi\|_{\mathcal{Y}}^2)\\ &= \|\varphi\|_{\mathcal{Y}}^2\mathbf{E}(\|\Sigma\|_{\mathcal{Y}}^2) < \infty\end{aligned}$$

for any $\varphi \in \mathcal{Y}$. From the following example we can see that the converse is not true, i.e. a white noise process cannot always be written as a Hilbert-space valued random variable with finite second moments. In order to prove this, we consider $\mathcal{Y} = l^2(\mathbf{N})$, the set of all sequences of real numbers $(f_i)_{i\in\mathbf{N}}$ such that $\sum_{i=1}^{\infty} f_i^2 < \infty$ and we choose the orthonormal system $(e_i)_{i\ge 1}$ in $l^2(\mathbf{N})$ given by

$$e_i = (0,\cdots,0,1,0,\cdots)$$

with 1 on the i-th position. If $(\varepsilon_i)_{i\ge1}$ is a sequence of independent Gaussian random variable with mean 0 and variance 1, we define the white noise process ϵ as

$$\epsilon : l^2(\mathbf{N}) \to L^2(\Omega,\mathcal{K},\mathbf{P}), \quad \epsilon(\varphi) := \sum_{i=1}^{\infty}\varphi_i\varepsilon_i.$$

Since $\mathbf{cov}(\varepsilon_i,\varepsilon_j) = \delta_{i,j}$ it follows that

$$\begin{aligned}\mathbf{E}\left\langle \varphi,\epsilon\right\rangle &= \mathbf{E}\left(\sum_{i=1}^{\infty}\varphi_i\varepsilon_i\right) = \sum_{i=1}^{\infty}\varphi_i\mathbf{E}(\varepsilon_i) = 0,\\ \left\langle \mathbf{cov}_{\varepsilon}\varphi_1,\varphi_2\right\rangle_{l^2(\mathbf{N})} &= \mathbf{cov}(\left\langle\varepsilon,\varphi_1\right\rangle,\left\langle\varepsilon,\varphi_2\right\rangle)\\ &= \mathbf{cov}(\sum_{i=1}^{\infty}\varphi_{1,i}\epsilon_i,\sum_{j=1}^{\infty}\varphi_{2,j}\epsilon_j)\\ &= \sum_{i,j=1}^{\infty}\varphi_{1,i}\varphi_{2,j}\mathbf{cov}(\varepsilon_i,\varepsilon_j)\\ &= \sum_{i,j=1}^{\infty}\varphi_{1,i}\varphi_{2,j}\delta_{i,j}\\ &= \sum_{i=1}^{\infty}\varphi_{1,i}\varphi_{2,i}\\ &= \left\langle\varphi_1,\varphi_2\right\rangle_{l^2(\mathbf{N})}\end{aligned}$$

for all $\varphi,\varphi_1,\varphi_2 \in l^2(\mathbf{N})$ and this implies that ϵ is a white noise process. If we could identify ϵ with a Hilbert-space valued random variable with second order moments, we should have $\epsilon : (\Omega,\mathcal{K},\mathbf{P}) \to l^2(\mathbf{N})$ but the second moment cannot be finite as

$$\mathbf{E}\|\epsilon\|_{l^2(\mathbf{N})}^2 = \mathbf{E}\sum_{i=1}^{\infty}|\varepsilon_i|^2 = \sum_{i=1}^{\infty}\mathbf{E}|\varepsilon_i|^2 = \sum_{i=1}^{\infty}1 = \infty.$$

From now on we assume the noise model (2.3) with ϵ a Hilbert-space process such that $\|\mathbf{cov}_\epsilon\| \le 1$ and $\mathbf{E}\epsilon = 0$.
In the next paragraphs we discuss the criteria of optimality used in statistical inverse problems and compare them with the deterministic setting.

2.2 Optimality for deterministic inverse problems

In this section we assume that Y^δ is the noisy data

$$Y^\delta = F(a^\dagger) + \delta\xi \tag{2.4}$$

satisfying $\|Y^\delta - u^\dagger\| \le \delta$ in the noise model (2.3) with deterministic level noise δ. Since we assumed that the operator F is ill-posed, regularization of the problem is required.
In general terms, regularization is the approximation of an ill-posed problem by a family of neighboring well-posed problems. We define a regularization method as a parametrized family of bounded operators R_α with the property of pointwise convergence as $\alpha \to 0$

$$\lim_{\alpha\to 0} R_\alpha F\varphi = \varphi$$

for all $\varphi \in \mathcal{Y}$, for the parameter α is chosen accordingly to a specific rule with respect to the noise level δ and the data Y^δ (see [EHN96]). The literature regarding regularization methods is huge, we quote here only a few references (see eg. [EHN96, Kir96]). Formally, a **regularization scheme** for an injective operator $F : \mathcal{X} \to \mathcal{Y}$ is a family of continuous operators $R_\alpha : \mathcal{Y} \to \mathcal{X}$, $\alpha \in (0, \alpha_0]$ such that for all $u^\dagger = F(a^\dagger) \in R(F)$ there exists a parameter choice rule $\alpha = \alpha(\delta, \widehat{u})$ such that the **worst case error** for noise level δ

$$\Delta_R(\delta, u^\dagger, F) = \sup\left\{\|R_{\alpha(\delta,Y^\delta)}Y^\delta - a^\dagger\| : Y^\delta \in \mathcal{Y}, \|Y^\delta - u^\dagger\| \le \delta\right\} \tag{2.5}$$

converges to 0 when $\delta \to 0$

$$\lim_{\delta\to 0} \Delta_R(\delta, u^\dagger, F) = 0. \tag{2.6}$$

Here, the regularization parameter choice

$$\alpha : \mathbf{R}_+ \times \mathcal{Y} \to (0, \alpha_0)$$

is such that

$$\lim_{\delta\to 0} \sup\left\{\alpha(\delta, Y^\delta) : Y^\delta \in Y, \|Y^\delta - u^\dagger\| \le \delta\right\} = 0. \tag{2.7}$$

A pair (R_α, α) is called a (convergent) **regularization method** (for solving $Fa^\dagger = u^\dagger$) if (2.6) and (2.7) hold. The choice of the regularization parameter is called **a-priori** parameter choice if it doesn't depend on Y^δ, but only on δ, otherwise we call it an **a-posteriori** parameter choice rule. In the deterministic case, a result due to Bakushinskii shows that a parameter choice rule depending only on Y^δ and not on δ cannot be a part of a convergent regularization method in the sense of our definition. The choice of the regularization parameter is fundamental for the accuracy of the estimator, as we are going to see in the section dedicated to Tikhonov regularization for nonlinear inverse problems. A measure of the quality of the estimator is the rate with which

$$\|a_\alpha^\delta - a^\dagger\| \to 0 \text{ as } \delta \to 0$$

where $a_\alpha^\delta = R_{\alpha(\delta, Y^\delta)} Y^\delta$. A uniform convergence rate for a regularization method does not exist if $R(F)$ is non-closed, i.e. the convergence is arbitrarily slow (see [EHN96]). Convergence rates can be given only on subsets of $D(F)$, this means under a-priori assumptions on the exact data. These assumptions are usually formulated with the help of a smoothing operator B of the form

$$\{x \in \mathcal{X} : x = Bw, \|w\| \leq \rho\}.$$

A condition of the form

$$a^\dagger = f(B)w, w \in \mathcal{X}, \|w\| \leq \rho$$

with a continuous function f with $f(0) = 0$ is called a **source condition**. The most common choice is

$$\begin{aligned} f(\lambda) &= \lambda^\mu \\ B &= F'(a^\dagger)^* F'(a^\dagger) \end{aligned}$$

with $\mu > 0$, which leads to **Hölder type smoothness conditions** and to the source sets

$$\begin{aligned} X_{\mu,\rho} &= \{x \in \mathcal{X} : x = (B^*B)^\mu w, \|w\| \leq \rho\} \\ X_\mu &= \bigcup_{\rho > 0} X_{\mu,\rho} = R((B^*B)^\mu). \end{aligned}$$

In her paper about weighted cross-validation for Tikhonov regularization in statistical linear inverse problems Wahba used for the first time the notions of degree of ill-posedness and source conditions, expressed in terms of rates of decay of the singular values of the operator and of the the exact data (see [Wah77]). The degree of ill-posedness is a term which she invented to quantify the interplay between the 'nastiness' of operator F and the effective smoothness of the regularizing set X_μ (see [NP99]). For a compact operator F the degree of ill-posedness is given by the rate of decay of its singular values σ_n. If they decay with order $n^{-\alpha}$, $\alpha \in \mathbf{R}_+$ we call the problem **mildly-ill posed**, otherwise we have a **severely ill-posed** problem, for example if the order is $\mathcal{O}\left(e^{-n}\right)$. We define now the optimality notions which we are going to use in the next chapters. If the worst case error

$$\Delta_R(\delta, X_{\mu,\rho}, F) = \sup\left\{\|R_{\alpha(\delta,Y^\delta)}\left(Y^\delta\right) - a^\dagger\| : Y^\delta \in \mathcal{Y}, \|Y^\delta - Fa^\dagger\| \le \delta, a^\dagger \in X_{\mu,\rho}\right\}$$

is minimal (for all $\delta > 0$) under all possible regularization methods we would have the natural and strongest optimality criterium for a regularization method. Since for some δ

$$\inf_R \Delta_R(\delta, X_{\mu,\rho}, F) = \rho^{\frac{1}{2\mu+1}} \delta^{\frac{2\mu}{2\mu+1}}$$

if F is linear, another weaker notion of optimality will be used (see [EHN96]).

Definition 2.1. *Let F be linear, $R(F)$ non-closed and let $\{R_\alpha\}$ be a regularization scheme for F. For $\mu, \rho > 0$ and $u^\dagger \in FX_{\mu,\rho}$, let α be a parameter choice rule for solving $Fa^\dagger = u^\dagger$. We call (R_α, α) optimal in $X_{\mu,\rho}$ if*

$$\Delta_R(\delta, X_{\mu,\rho}, F) = \delta^{\frac{2\mu}{2\mu+1}} \rho^{\frac{1}{2\mu+1}} \tag{2.8}$$

holds for all $\delta > 0$.
We call (R_α, α) of optimal order in $X_{\mu,\rho}$ if there exists a constant $c \ge 1$ such that

$$\Delta_R(\delta, X_{\mu,\rho}, F) \le c\delta^{\frac{2\mu}{2\mu+1}} \rho^{\frac{1}{2\mu+1}}$$

holds for all $\delta > 0$.

In inverse problem literature the optimality of regularization methods is studied based on the notions presented in Definition 2.1. Another important concept in the study of optimality of the regularization methods is the **qualification**. Under the Hölder type source conditions $X_{\mu,\rho}$ and for a general regularization method (R_α, α), the qualification q_0 is defined as

$$q_0 = \sup_\mu \inf_\alpha \sup_{\delta>0} \Delta_R(\delta, X_{\mu,\rho}, F)\delta^{\frac{-2\mu}{2\mu+1}} < \infty.$$

We focus here on the Tikhonov regularization for which it can be easily seen that the qualification is 1. This implies that the best possible rate of convergence for Tikhonov regularization is $\delta^{\frac{2}{3}}$ and for $\mu > 1$ the saturation appears. That is why different methods to overcome this problem were developed, like iterated Tikhonov regularization or regularization in Hilbert scales. Rates of convergence for Tikhonov regularization have been studied for deterministic noise in [EKN89, Neu92, SEK93, TJ03], and for random noise in [BHM04, LL05, O'S90]. Tikhonov regularization in Hilbert scales is going to be the subject of the section 2.4.

2.3 Optimality in statistical inverse problems

We consider now the general noise model (2.3) with stochastic noise

$$Y = F(a^\dagger) + \sigma\epsilon \tag{2.9}$$

and we define measures of performance necessary to study the optimality of a non-parametric estimator in a statistical problem. A **consistent** estimator is an estimator that converges in probability to the quantity being estimated as the sample size grows. If the estimator converges almost surely to the exact value, we talk about **strong consistency**.
Consistency is the the statistical notion corresponding to convergence in the deterministic setting. The notion of convergence, corresponding to strong consistency is stronger than the consistency. We are looking to assess the quality of an estimator $\widehat{a}$ of $a^\dagger \in \mathcal{X}$ and we are going to use the expected square error

$$\mathrm{ESE} = \mathbf{E}\|a^\dagger - \widehat{a}\|^2_{\mathcal{X}}$$

where the mean $\mathbf{E}$ is taken with respect to the probability P_Y of Y. The mathematical simplicity of ESE, due also to the following bias-variance decomposition

$$\begin{aligned} \mathrm{ESE} &= \|\mathbf{E}(\widehat{a} - a^\dagger\|^2_{\mathcal{Y}} + \mathbf{Var}(\widehat{a}), \\ \mathbf{Var}(\widehat{u}) &= \mathbf{E}(\|\widehat{a} - \mathbf{E}(\widehat{a})\|^2_{\mathcal{Y}}) \end{aligned}$$

which holds for a linear R_α is one of the reasons why this risk function is used for measuring the global performance of the non-parametric estimators.
In order to choose the estimator with the smallest possible error we need to define some criterium which allows us to compare the quality of the estimation. We use the maximal risk to control uniformly the error over a given class of functions (see e.g. [Cav03]). This non-parametric class of functions contains the exact solution $a^\dagger$ and corresponds to the 'source sets' $\mathcal{X}_{\mu,\rho}$ in the deterministic case, for example $\mathcal{X}_{\mu,\rho}$ is a ball in a Hölder or Sobolev space.The asymptotical study of this risk as $\sigma \to 0$ allows us to quantify the quality of the estimator. A natural definition of the **maximal risk** in the noise model (2.9), corresponding to the worst case error in the deterministic case, is

$$\tilde{\Delta}_R(\sigma, \mathcal{X}_{\mu,\rho}, F) = \sup\left\{ \left(\mathbf{E}\|R_{\alpha(\sigma,Y)}(Y) - a^\dagger\|^2\right)^{\frac{1}{2}} : Y = F(a^\dagger) + \sigma\epsilon, a^\dagger \in \mathcal{X}_{\mu,\rho} \right\}$$

and the **minimax risk**, corresponding to the best possible order of accuracy in the deterministic model, is

$$\inf_R \tilde{\Delta}_R(\sigma, \mathcal{X}_{\mu,\rho}, F).$$

The minimax risk is the minimum over all estimators of maximum risk on a class $\mathcal{X}_{\mu,\rho}$. A **minimax estimator** $\widehat{a}$ attains exactly or approximately (up to

a constant) the minimax risk. The big problem of minimax estimators is that they depend on the smoothness of the exact data $a^\dagger$ which needs to be known to construct a minimax estimator. In the real world this is usually not known, but we still would like to be able to determine an estimator with the best speed of convergence possible, sometimes optimal, but which does not require a-priori knowledge of the smoothness of the solution. The methods which allow us to do this are called **adaptive methods**. Sometimes the adaptive estimators are optimal in the minimax sense but sometimes this is not possible (see e.g. [Lep92]). We will come back to the adaptive choice of the regularization parameter in the next chapters.
A large literature exists for ESE and minimax rates in the case of linear statistical inverse problems. We summarize first the results due to Pinsker (see [Pin80, Tsy04]). He obtained minimax rates for a **direct regression problem**

$$Y = a^\dagger + \sigma\epsilon$$

which coincides to the estimation problem (2.3) with the operator F the identity operator. Let $\{\varphi_k : k \in \mathbf{N}\}$ be an orthonormal basis of $\mathcal{X}$ and consider the subspaces

$$\mathcal{X}_{\mu,\rho} = \left\{ a \in \mathcal{X} : \sum_{k\in\mathbf{N}} |\left\langle a^\dagger, \varphi_k \right\rangle|^2_{\mathcal{X}} k^{2\mu} \leq \rho^2 \right\} \qquad \mu, \rho > 0$$

For these 'smoothness classes', Pinsker proved for the case that ϵ is Gaussian white noise that

$$\lim_{\sigma\to 0} \inf_{R} \sup_{a^\dagger\in\mathcal{X}_{\mu,\rho}} \sigma^{\frac{-2\mu}{2\mu+1}} \left(\mathbf{E}\|\widehat{a} - a^\dagger\|^2_{\mathcal{X}}\right)^{\frac{1}{2}} = C^* \tag{2.10}$$

where C^* is Pinsker's constant and can be computed knowing ρ and μ. The first step of our algorithm consists in the direct non-parametric estimation of the right hand side function $u^\dagger$, but our aim is to solve a statistical inverse problem, this means to estimate the indirectly observed function $a^\dagger$ which is connected to $u^\dagger$ with the help of the operator (1.1). This is an inverse non-parametric estimation problem. Minimax rates for linear statistical inverse problems with a more general operator than the identity were extensively studied. Lower bounds for a linear statistical inverse problem with Hermitian operator were obtained in [vRR96]. In the case of the indirect regression problem (2.9) with F compact and strictly positive self-adjoint operator with eigenvalues $\sigma_k \sim k^{-\nu}$ satisfies

$$\inf_{R} \sup_{a^\dagger\in\mathcal{X}_{\mu,\rho}} \mathbf{E}_{a^\dagger}\|\widehat{a} - a^\dagger\|^2_{\mathcal{X}} \geq c\sigma^{\frac{2\mu}{2\mu+2\nu+1}}.$$

with c a generic constant. Note that the lower bound depends on the operator, in contrast to the deterministic setting. The condition on the rate of decay for the eigenvalues of the operator F corresponds to a mildly ill-posed problem. While the linear statistical problems were widely studied (see e.g. [ES02] for a review), the nonlinear statistical inverse problems were studied until now only by Sullivan([O'S90]) and Bissantz, Hohage, Munk (see [BHM04]). The study of rates of convergence for nonlinear statistical inverse problems is the aim of our thesis.

2.4 Tikhonov regularization in deterministic nonlinear inverse problems

Let us consider now the nonlinear operator F as in (1.1). We assume that F is continuous and weakly sequentially closed, i.e. for any sequence $a_n \in D(F)$ that converges weakly to a in $\mathcal{X}$ and for which $F(a_n)$ converges weakly to u in $\mathcal{Y}$ it follows that $a \in \mathcal{X}$ and $F(a) = u$.
We are interested in solving the ill-posed operator equation (1.1) given noisy data $Y^\delta \in \mathcal{Y}$ as in the noise model (2.4). We assume that it exists $a^\dagger$ the exact solution corresponding to the exact data $u^\dagger$ and that F is locally injective in $a^\dagger$, i.e. $F(a) = u^\dagger$ implies $a = a^\dagger$. We replace the problem (1.1) by the minimization problem

$$\|F(a) - Y^\delta\|^2_{\mathcal{Y}} + \alpha\|a - a_0\|^2_{\mathcal{X}} \to \min, a \in D(F) \tag{2.11}$$

where $\alpha > 0$ is the regularization parameter and $a_0 \in \mathcal{X}$ is an initial guess. The choice $a_0 = 0$ has here no special role, in contrast to the linear case. Under the assumptions stated above there exists a global minimum a^δ_α for the Tikhonov functional

$$a \mapsto \|F(a) - Y^\delta\|^2_{\mathcal{Y}} + \alpha\|a - a_0\|^2_{\mathcal{X}} : D(F) \to \mathbf{R}. \tag{2.12}$$

The stability of the solution of problem (2.11) is proved in the following theorem (for details and proof see [EKN89]).

Theorem 2.2. *Let $\alpha > 0$ and let (u_k) and (a_k) be sequences where $u_k \to Y^\delta$ and a_k is a minimizer of 2.11 with Y^δ replaced by u_k. Then there exists a convergent subsequence of (a_k) and the limit of every convergent subsequence is a minimizer of (2.11).*

A detailed convergence analysis of this estimator is available also in [EHN96]. Under the same assumptions on the regularization parameter and the noise as in the linear case it was proved that the solutions of (2.11) converge to a a_0-solution of (1.1). We cite this result here.

Theorem 2.3. *Let $u^\dagger \in \mathcal{Y}$ with $\|Y^\delta - u^\dagger\| \le \delta$ and let $\alpha(\delta)$ be such that $\alpha(\delta) \to 0$ and $\frac{\delta^2}{\alpha(\delta)} \to 0$ as $\delta \to 0$. Then every sequence $a^{\delta_k}_{\alpha_k}$, where $\delta_k \to 0$, $\alpha_k = \alpha(\delta_k)$*

and $a_{\alpha_k}^{\delta_k}$ is a solution to 2.11, has a convergent subsequence. The limit of every convergent subsequence is an a_0-minimum norm solution. If in addition, the a_0-minimum norm solution a_α^δ is unique, then

$$\lim_{\delta \to 0} a_\alpha^\delta = a^\dagger.$$

In other words, Tikhonov regularization is a convergent regularization method. In the linear case Tikhonov regularization has qualification equal to 1 and saturation is achieved at the rate $\mathcal{O}(\delta^{\frac{2}{3}})$, where this rate is obtained under the source condition $a^\dagger - a_0 \in R(F^*F)$ (see [Gro84]). In the nonlinear case, Neubauer proved that Tikhonov regularization method saturates at the same rate under the smoothness condition $a^\dagger - a_0 \in R(F'(a^\dagger)^* F'(a^\dagger))$ (see [Neu89]). The order optimal rates of convergence are also known, as we can see from the next theorem ([EHN96]).

Theorem 2.4. *Let $D(F)$ be convex and $a^\dagger$ be an element in the interior of $D(F)$. If it holds:*

1. *F is Fréchet differentiable,*
2. *there exists $L \leq 0$ such that $\|F'(a^\dagger) - F'(a)\| \leq L\|a^\dagger - a\|$ for all $a \in D(F)$ in a sufficiently large ball around $a^\dagger$,*
3. *$a^\dagger - a = (F'(a^\dagger)^* F'(a^\dagger))^\mu v$, for some $\mu \in [\frac{1}{2}, 1]$*
4. *$L\|v\| < 1$*

then, for the choice $\alpha \sim \delta^{\frac{2}{2\mu+1}}$, we obtain

$$\|a_\alpha^\delta - a^\dagger\| = \mathcal{O}(\delta^{\frac{2\mu}{2\mu+1}}).$$

The source condition 3 with $\mu = \frac{1}{2}$ is critical for the study of the nonlinear Tikhonov regularization. The degree of nonlinearity defined in [HS94] characterizes the relations between the remainder of a formal Taylor series expansion of F in a neighborhood of $a^\dagger$ $\|F(a) - F(a^\dagger) - F'(a^\dagger)(a - a^\dagger)\|$ and the linear part $\|F'(a^\dagger)(a^\dagger - a)\|$, the increments of values, respectively the increments of arguments $\|F(a) - F(a^\dagger)\|$ and $\|a - a^\dagger\|$. On the other hand, the local degree of ill-posedness in $a^\dagger$, υ, is evaluated with the help of the nullspace and the decay rate of the singular values of $F'(a^\dagger)$

$$\upsilon = \sup\left\{\mu : \sigma_i = \mathcal{O}\left(\frac{1}{i^\mu}\right), \sigma_i \text{ eigenvalues of } F'(a^\dagger)\right\}.$$

For the case $\mu < \frac{1}{2}$ order optimal rates of convergence were proved in [HS94] under stronger conditions related to the local degree of ill-posedness for nonlinear problems and under a-priori choice of the regularization parameter. The connection between the degree of nonlinearity and the local degree of the ill-posedness in $a^\dagger$ is used to analyse the rates of convergence under Hölder type source conditions and for the choice of the regularization parameter α of order $\delta^{\frac{2}{1+2\mu}}$ for $\mu < \frac{1}{2}$.

2.5 Tikhonov regularization in statistical nonlinear inverse problems

In this section we consider the problem (1.1) in the statistical setting (2.9) with stochastic noise level σ. We assume in a first step that an estimator $\widehat{u}$ of $u^\dagger$ with known ESE β is at our disposal, as suggested in [BHM04]. On the second step we estimate $a^\dagger$ from $\widehat{u}$ using nonlinear Tikhonov regularization or Method of Regularization. We choose the estimator $\widehat{a}$ as a solution of the least squares problem:

$$\widehat{a} := \operatorname{argmin}_{a \in D(F)} \left(\|F(a) - \widehat{u}\|_{\mathcal{Y}}^2 + \alpha \|a - a_0\|_{\mathcal{X}}^2 \right) \tag{2.13}$$

Here $a_0 \in \mathcal{X}$ denotes also some initial guess of $a^\dagger$, which offers the possibility to incorporate a-priori information. The estimators (2.13) arise naturally in a Bayesian description of the problem (see [KS04]). The first step in the study of a statistical estimator is to check its consistency, which is the notion corresponding to the deterministic convergence (see paragraph (2.3)). It follows from [BHM04] that the method is consistent in the sense that for any choice of minimizing elements $\widehat{a} \in D(F)$ we have

$$\mathbf{E}\|\widehat{a} - a^\dagger\|_{\mathcal{X}}^2 \to 0 \tag{2.14}$$

if $\alpha \to 0$ and $\beta^2/\alpha \to 0$. We cite here this result.

Theorem 2.5. *Assume that F is a nonlinear, one-to-one (in the sense defined above), weakly sequentially closed operator and $\widehat{u}$ is an estimator of $u^\dagger$ such that (1.5) holds. Let $\widehat{a}$ denote a (not necessarily unique) solution to the minimization problem (2.13) and assume that the regularization parameters $\alpha > 0$ are chosen such that*

$$\alpha \to 0, \frac{\beta^2}{\alpha} \to 0 \ \textit{as}\ \beta \to 0.$$

Then

$$\mathbf{E}\|\widehat{a} - a^\dagger\|_{\mathcal{X}}^2 \to 0, \ \textit{as}\ \beta \to 0.$$

In particular, it was shown in [BHM04] that the estimators (2.13) converge with the rate

$$\sqrt{\mathbf{E}\|\widehat{a} - a^\dagger\|_{\mathcal{X}}^2} = \mathcal{O}\left(\sqrt{\beta}\right) \tag{2.15}$$

for the choice $\alpha \sim \beta$ if F has a Fréchet derivative F' which is Lipschitz continuous with constant L and if there exists $w \in \mathcal{Y}$ such that

$$a^\dagger - a_0 = F'[a^\dagger]^* w \qquad \text{and} \qquad L\|w\|_{\mathcal{Y}} < 1. \tag{2.16}$$

This rate of convergence coincides with the one in the deterministic case. To improve this results we will make a short excursion in functional analysis in the next chapter in order to present some basic properties of Hilbert scales.

Chapter 3

Self-adjoint operators and Hilbert scales

Hilbert scales are defined with the help of self-adjoint operators. We review in the following chapters some general properties of these operators. In Chapter 6 we consider operators defined in Hilbert scales and the notion of Gelfand triple, which is shortly presented in the first section, is very useful to study the properties of these operators. Friedrichs extension is a possibility to construct a self adjoint operator and we present it here, together with examples. Afterwards, we study properties of Hilbert scales and we use Friedrichs extension to generate Hilbert scales. Finally, we survey optimality results for Tikhonov regularization in Hilbert scales for linear inverse problems.

3.1 General properties of self-adjoint operators

We present now some properties of the self-adjoint operators which are very useful for our study of Hilbert scales in the following sections. The notion of adjoint of an operator generalizes the conjugate transpose of a matrix to the infinite-dimensional situation. If we consider a linear operator between two Hilbert spaces, we can define the Hilbert adjoint of this operator.

Definition 3.1. *Let $(D(A), A)$ be a densely defined linear operator from a Hilbert space $\mathcal{X}$ to a Hilbert space $\mathcal{Y}$. We define $D(A^*)$ to be the set of all $v \in \mathcal{Y}$ such that there exists $w \in \mathcal{X}$ which fulfills*

$$\langle v, Au \rangle_{\mathcal{Y}} = \langle w, u \rangle_{\mathcal{X}} \tag{3.1}$$

for all $u \in D(A)$. As $D(A)$ is dense, w is uniquely determined by $v \in D(A^*)$ and (3.1). We can define an operator $(D(A^*), A^*)$ from $\mathcal{Y}$ to $\mathcal{X}$ by

$$A^* v = w$$

*for every $v \in D(A^*)$. We call $(D(A^*), A^*)$ the **(Hilbert) adjoint** of $(D(A), A)$.*

Example 3.2. *Let us consider the integral linear operator*

$$A : L^2(0,1) \to L^2(0,1), \quad (Af)(t) := \int_0^1 k(t,s)f(s)\,ds$$

where $k : [0,1] \times [0,1] \to \mathbf{R}$ *is an* L^2*-kernel, i.e.* $\int_0^1 \int_0^1 |k(x,t)|^2\,dx\,dt < \infty$ *and* $\overline{u}$ *is the complex conjugate of* u*. Then operator* A *is bounded and compact (see e.g. [PS90]). The adjoint of* A

$$A^* v(t) = \int_0^1 \overline{k(s,t)} v(s)\,ds.$$

is defined on $L^2(0,1)$*, also has an* L^2*-kernel and, in general, does not coincide with* A*. In our application for Hammerstein operator in Chapter 6 we consider the operator* $A = \int_0^t f(s)\,ds$ *with the* L^2*-kernel*

$$k(t,s) = \mathcal{I}_{[0,t]}(s).$$

which is the characteristic function of the interval $[0,t]$*. Then the adjoint is given by*

$$A^* f(t) = \int_t^1 f(s)\,ds.$$

We state here some properties of the adjoint of an operator (for proofs see e.g.[Wer95]).

Proposition 3.3. *Let* $A : D(A) \subseteq \mathcal{X} \to \mathcal{Y}$ *and* $B : D(B) \subseteq \mathcal{X} \to \mathcal{Y}$ *be linear operators, where* $D(A)$ *and* $D(B)$ *are dense in the Hilbert space* $\mathcal{X}$ *over the field* K*. Then, the following hold true:*
1. For each $\alpha \in K$*,*

$$(\alpha A)^* = \overline{\alpha} A^*.$$

2. If B *is an extension of* A *(i.e.* $D(A) \subseteq D(B), A = B\,|_{D(A)}$*) then* A^* *is an extension of* B^**.*
3. The orthogonal complement of the range of A *is the nullspace of the adjoint*

$$R(A)^\perp = N(A^*).$$

4. The closure of the range of A *is the orthogonal complement of the nullspace of* A^*

$$\overline{R(A)} = (\ker A^*)^\perp.$$

5. If $S \in L(\mathcal{X}, \mathcal{Y})$ *and* $T \in L(\mathcal{Y}, \mathcal{Z})$ *then*

$$(TS)^* = S^* T^*$$

for any Hilbert spaces $\mathcal{X}$*,* $\mathcal{Y}$ *and* $\mathcal{Z}$*.*

First we remind of the definition of a Gelfand triple $V \subseteq \mathcal{X} \subseteq V'$.

Definition 3.4. *A triple of Hilbert spaces* $(V, \mathcal{X}, V')$ *is named* ***Gelfand triple*** *if* V *is dense in* $\mathcal{X}$ *and* $V \hookrightarrow \mathcal{X} \hookrightarrow V'$ *are continuous embeddings.*

Actually, a Gelfand triple consists of a Hilbert space $\mathcal{X}$, together with a densely embedded (in the $\mathcal{X}$-norm) subspace V which carries a finer topology, that is one for which the natural inclusion $V \subseteq \mathcal{X}$ is continuous. The restriction to V of a linear and bounded functional $f \in \mathcal{X}'$ is a linear and bounded functional on V and $\mathcal{X}'$ is continuously embedded in V'. Now, by the Riesz representation theorem we can identify $\mathcal{X}'$ with $\mathcal{X}$. Therefore the definition of a Gelfand triple space is in terms of a sandwich: $V \subseteq \mathcal{X} \subseteq V'$ (see e.g. [Ruz95]). Any vector $u \in \mathcal{X}$ is a linear functional in V'

$$v \mapsto \langle u, v \rangle_{\mathcal{X}}\,,\ v \in V$$

with norm

$$\|u\|_{V'} := \sup_{v \in V\setminus\{0\}} \frac{|\langle u, v \rangle_{\mathcal{X}}|}{\|v\|_V}.$$

The inner product on $\mathcal{X}$ can be extended to a continuous, sesquilinear function

$$\langle \cdot, \cdot \rangle_{\mathcal{X}} : V \times V' \to K$$

with

$$|\langle v, u \rangle_{\mathcal{X}}| \leq \|v\|_V \|u\|_{V'},\ u \in V', v \in V. \tag{3.2}$$

Hence, for any $u \in V$ there exist two different functionals in V', $v \mapsto \langle u, v \rangle_V$ and $v \mapsto \langle u, v \rangle_{\mathcal{X}}$. An example of Gelfand triple is the embedding of Sobolev spaces of functions defined on a smooth domain Ω $(H_0^1(\Omega), L^2(\Omega), H^{-1}(\Omega))$. The next lemma is going to be repeatedly used in Chapter 4.

Lemma 3.5. *Let* $V_j \subset \mathcal{X}_j \subset V_j'$ *(* $j = 1, 2$*) be Gelfand triples and* $A \in L(V_1, V_2)$*. Then there exists a unique Gelfand-adjoint* $A' \in L(V_2', V_1')$ *satisfying*

$$\langle A\varphi_1, \varphi_2 \rangle_{\mathcal{X}_2} = \langle \varphi_1, A'\varphi_2 \rangle_{\mathcal{X}_1} \tag{3.3}$$

for all $\varphi_1 \in V_1$ *and* $\varphi_2 \in V_2'$*. Moreover*

$$\|A\|_{V_2 \leftarrow V_1} = \|A'\|_{V_1' \leftarrow V_2'}. \tag{3.4}$$

and, if A *has a bounded inverse* $A^{-1} : V_2 \to V_1$*, then* $(A^{-1})' = (A')^{-1}$ *and*

$$\|A^{-1}\|_{V_1 \leftarrow V_2} = \|\left(A^{-1}\right)'\|_{V_2' \leftarrow V_1'}. \tag{3.5}$$

Proof. Let us consider the linear operators $E_{V_j} : V_j' \to V_j, j = 1, 2$ which are uniquely determined by

$$\langle x, y \rangle_{\mathcal{X}_j} = \left\langle E_{V_j} x, y \right\rangle_{V_j}$$

for all $x \in V', y \in V$. Since for $x \in \mathcal{X}_j$ we have that

$$\|E_{V_j} x\|_{V_j} = \sup_{y \in V_j \setminus \{0\}} \frac{\langle x, y \rangle_{\mathcal{X}_j}}{\|y\|_{V_j}} = \|x\|_{V_j'}$$

and, as $\mathcal{X}_j$ is dense in V_j', the operator E_{V_j} is unitary. Since

$$\begin{aligned}
\langle A\varphi_1, \varphi_2 \rangle_{\mathcal{X}_2} &= \langle A\varphi_1, E_{V_2}\varphi_2 \rangle_{V_2} \\
&= \langle \varphi_1, A^* E_{V_2}\varphi_2 \rangle_{V_1} \\
&= \left\langle \varphi_1, E_{V_1^*} A^* E_{V_2}\varphi_2 \right\rangle_{\mathcal{X}_1} \\
&= \langle \varphi_1, A'\varphi_2 \rangle_{\mathcal{X}_1} .
\end{aligned}$$

for all $\varphi_1 \in V_1, \varphi_2 \in V_2'$. It follows that the Gelfand-adjoint A' exists and is given by

$$A' = E_{V_1}^* A^* E_{V_2}.$$

The first norm equality follows immediately, since $E_{V_j}, j = 1, 2$ are unitary operators. If A has a bounded inverse A^{-1} then

$$\begin{aligned}
\left(A^{-1}\right)' &= E_{V_2}^* \left(A^{-1}\right)^* E_{V_1} \\
&= E_{V_2}^* \left(A^*\right)^{-1} E_{V_1} \\
&= \left(A'\right)^{-1}
\end{aligned}$$

and (3.5) follows using again the unitarity of $E_{V_j}, j = 1, 2$. □

Definition 3.6. *An operator $(D(A), A)$ from the Hilbert space $\mathcal{X}$ to $\mathcal{X}$ with dense domain $D(A)$ is said to be **symmetric** if $(D(A^*), A^*)$ is an extension of $(D(A), A)$, this means if*

$$\langle Au, v \rangle = \langle u, Av \rangle$$

for every $u, v \in D(A)$.

Definition 3.7. *An operator is said to be **self-adjoint** if*

$$(D(A), A) = (D(A^*), A^*).$$

The self-adjoint operators can be seen as generalization of Hermitian matrices in (possibly) infinite-dimensional spaces. An operator is self-adjoint if and only if it is symmetric and $D(A) = D(A^*)$. As a consequence of the closed graph theorem unbounded operators are self-adjoint only if they are defined on a strict subset of the Hilbert space $\mathcal{X}$, because self-adjoint operators are closed. In particular, a symmetric, everywhere defined operator is self-adjoint and it is also a bounded operator. We study now the relation between symmetry and self-adjointness for unbounded operators (see e.g. [Tay96a]).

Lemma 3.8. *Let $A : \mathcal{X} \to \mathcal{X}$ be a self-adjoint and injective operator. Then $A^{-1} : R(A) \to \mathcal{X}$ is a self-adjoint operator.*

Proof. As the operator $A : \mathcal{X} \to R(A) \subseteq \mathcal{X}$ is injective and self-adjoint, the operators $A^{-1} : R(A) \subseteq \mathcal{X} \to \mathcal{X}$ and $(A^*)^{-1} : R(A^*) = R(A) \subseteq \mathcal{X} \to \mathcal{X}$ exist. Since $\overline{R(A)} = N(A^*)^{\perp} = N(A)^{\perp} = \mathcal{X}$, A^{-1} is densely defined in $\mathcal{X}$ and the operator $(A^{-1})^*$ also exists. Let us define the unitary mappings

$$\begin{aligned} U &: \mathcal{X} \times \mathcal{X} \to \mathcal{X} \times \mathcal{X}, \quad U(u, v) = (v, -u) \\ V &: \mathcal{X} \times \mathcal{X} \to \mathcal{X} \times \mathcal{X}, \quad V(u, v) = (v, u). \end{aligned}$$

We want to prove that $G((A^{-1})^*) = G((A^*)^{-1})$ where

$$G(A) = \{(u, Au) : u \in \mathcal{X}\}.$$

We notice that

$$G(A)^{\perp} = \{(u, v) \in \mathcal{X} \times \mathcal{X} : \langle (u, v), (f, Af) \rangle = 0, \forall (f, Af) \in G(A)\}.$$

and

$$\begin{aligned} G(A^*) &= \{(u, v) \in \mathcal{X} \times \mathcal{X} : \langle u, Af \rangle = \langle v, f \rangle, \forall f \in D(A)\} \\ &= \{(u, v) \in \mathcal{X} \times \mathcal{X} : \langle (u, v), (Af, -f) \rangle = 0, \forall (f, Af) \in G(A)\} \\ &= (U(G(A)))^{\perp} = U(G(A)^{\perp}) \end{aligned}$$

Moreover

$$G(A^{-1}) = V(G(A)).$$

Since $UV = -VU$ we have

$$\begin{aligned} G(\left(A^{-1}\right)^*) &= U\left(G(A^{-1})^{\perp}\right) \\ &= UV\left(G(A)^{\perp}\right) \\ &= VU(G(A)^{\perp}) \\ &= VG(A^*) \\ &= G\left((A^*)^{-1}\right) \\ &= G(A^{-1}) \end{aligned}$$

Therefore, A^{-1} is self-adjoint.
The next result, which we will need in Chapter 6, is proved with the help of Lemma 3.8.

Lemma 3.9. *Let $A : D(A) \subseteq \mathcal{X} \to \mathcal{X}$ a symmetric operator with $R(A) = \mathcal{X}$. Then A is self-adjoint.*

Proof. Because $R(A) = \mathcal{X}$ and $R(A^*) \supseteq R(A)$ it follows that $R(A^*) = \mathcal{X}$. From the properties of the adjoint, we have that $\ker A = \{0\}$ and, as A is injective, $A^{-1} : \mathcal{X} \to \mathcal{X}$ is well-defined. For $f, g \in \mathcal{X}$ there exist $u, v \in D(A)$ such that $f = Au$ and $g = Av$. Then, we have that

$$\left\langle A^{-1}f, g\right\rangle = \left\langle A^{-1}Au, Av\right\rangle = \langle u, Av\rangle = \langle Au, v\rangle = \left\langle f, A^{-1}g\right\rangle$$

which means that the operator A^{-1} is symmetric and defined on the whole space $\mathcal{X}$, so, A^{-1} is bounded and self-adjoint. We can apply now the previous Lemma to our self-adjoint and injective operator A^{-1} to obtain that A is self-adjoint. □
We will give now another useful result, due to J. von Neumann ([Tay96a]).

Lemma 3.10. *If $A : D(A) \subseteq \mathcal{X}_0 \to \mathcal{X}_1$ is closed and densely defined operator between the Hilbert spaces $\mathcal{X}_0$ and $\mathcal{X}_1$, then A^*A is self-adjoint and $I + A^*A$ has a bounded inverse.*

The construction of a self-adjoint operator due to Friedrichs (Friedrichs extension) is strongly related to the generation of Hilbert scales, as we are going to see in the next chapters. For now we are just presenting the theoretical aspects and let the applications for later. We start with an operator $j : \mathcal{X}_1 \hookrightarrow \mathcal{X}_0$,which is a continuous injection with dense range between two Hilbert spaces $\mathcal{X}_0$ and $\mathcal{X}_1$. The following theorem holds then true (see e.g. [Wei76]).

Theorem 3.11. *Let $j : \mathcal{X}_1 \to \mathcal{X}_0$ be a continuous injection with dense range defined between the two Hilbert spaces $(\mathcal{X}_0, \|\cdot\|_0)$ and $(\mathcal{X}_1, \|\cdot\|_1)$. Then there exists a unique self-adjoint operator $A : D(A) \subseteq \mathcal{X}_0 \to \mathcal{X}_0$ such that $D(A) \subseteq j(\mathcal{X}_1)$ and*

$$\langle Aj(u), j(v)\rangle_0 = \langle u, v\rangle_1 \tag{3.6}$$

for all $\{u : j(u) \in D(A)\}$ and $v \in \mathcal{X}_1$.

Proof. The proof follows the ideas from [Tay96a]. First, we define the operator A as

$$\begin{aligned} &D(A) = \{j(u) : u \in \mathcal{X}_1, \exists \overline{u} \in \mathcal{X}_0 \text{ such that } \langle u, v\rangle_1 = \langle \overline{u}, j(v)\rangle_0 \, \forall v \in \mathcal{X}_1\} \\ &Aj(u) = \overline{u}. \end{aligned}$$

A is well-defined because $\mathcal{X}_1$ is dense in $\mathcal{X}_0$ and, as a consequence, the element $\overline{u}$ is unique. It follows also that A is linear. Rewriting the definition of the domain $D(A)$ we get that

$$\langle Aj(u), j(v)\rangle_0 = \langle u, v\rangle_1 = \langle j^*Aj(u), v\rangle_1$$

so there exists $w \in \mathcal{X}_0$ such that $u = j^*(w)$. It follows that $D(A) = R(jj^*)$ and that for all $w \in \mathcal{X}_0$ and $v \in \mathcal{X}_1$ it holds

$$\langle Ajj^*(w), j(v)\rangle_0 = \langle j^*w, v\rangle_1 = \langle w, j(v)\rangle_0 .$$

This means that $A = (jj^*)^{-1}$. We remark that j is a closed operator because from $u_n \to u$ in $\|\cdot\|_1$-norm and $u_n \to w$ in $\|\cdot\|_0$-norm for a sequence $u_n \in D(j) = \mathcal{X}_1$ it follows that $u_n \to u$ in $\|\cdot\|_1$-norm and that $u = w \in D(j)$. Then j^* it is densely defined in $(\mathcal{X}_1, \|\cdot\|_1)$ and from the lemma due to von Neumann jj^* is self-adjoint. This means that A is a self-adjoint operator. Any other operator B which fulfills the conditions of the theorem is a restriction of A and, as it is also self-adjoint and $D(B) \subseteq D(A) \subseteq D(B^*)$, we have also the uniqueness of A. □

Remark 3.12. *We remark that, given a closed, densely defined operator A on $\mathcal{X}_0$, one can make $D(A) = \mathcal{X}_1$ a Hilbert space with inner product $\langle u, v\rangle_1 = \langle Au, Av\rangle_0 + \langle u, v\rangle_0$. Thus, Friedrich's result contains von Neumann's result.*

Remark 3.13. *If A is obtained by the Friedrich's extension method, from [Tay96b] we have*

$$D(A^{\frac{1}{2}}) = j(\mathcal{X}_1) \subseteq \mathcal{X}_0.$$

Proof. $D(A^{\frac{1}{2}})$ consists of elements of $\mathcal{X}_0$ which are limits of sequences in $D(A)$, in the norm $\|A^{\frac{1}{2}}u\|_{\mathcal{X}_0} + \|u\|_{\mathcal{X}_0}$. As shown in the previous proof, $D(A) = R(jj^*)$. Now

$$\|A^{\frac{1}{2}}jj^*(f)\|^2_{\mathcal{X}_0} = \langle Ajj^*(f), jj^*(f)\rangle_{\mathcal{X}_0} = \|j^*f\|^2_{\mathcal{X}_1}.$$

Thus a sequence $(jj^*(f_n))$ converges in the $D(A^{\frac{1}{2}})$-norm (to an element g) if and only if $(j^*(f_n))$ converges in $\mathcal{X}_1$-norm (to an element u) and $g = j(u)$. Since $j^* : \mathcal{X}_0 \to \mathcal{X}_1$ has dense range, all elements $u \in \mathcal{X}_1$ are the limit of such sequences $(j^*(f_n))$ and the proposition is proved. □

3.2 Sobolev spaces and examples of unbounded self-adjoint operators

We give now the definition of the Sobolev spaces, which we are going to use during our thesis.

Definition 3.14. *Let $\Omega \subseteq \mathbf{R}^m$, $m \in \mathbf{N}$ be open and let k be a non-negative integer. We define the Sobolev space $H^k(\Omega)$ to be the set of all distributions $u \in L^2(\Omega)$ such that the weak derivative $D^\alpha u \in L^2(\Omega)$ for all $|\alpha| \leq k$. In $H^k(\Omega)$,* *we define a norm and an inner product by*

$$\|u\|^2_{H^k(\Omega)} = \sum_{|\alpha|\le k} \|D^\alpha u\|^2,$$
$$\langle u, v\rangle_{H^k(\Omega)} = \sum_{|\alpha|\le k} \int_\Omega D^\alpha \overline{u(x)} D^\alpha v(x)\, dx.$$

The space $H^k(\Omega)$ defined above is a Hilbert space. In the next chapters we will also need the following definition.

Definition 3.15. *Under the assumptions from (3.14) we define $H_0^k(\Omega)$ to be the closure of the infinite differentiable functions $C_0^\infty(\Omega)$ in the $H^k(\Omega)$.*

Remark 3.16. *An equivalent definition of the Sobolev spaces, implying the use of the Fourier transform and which allows $k \in \mathbf{R}_+$, is also possible. We will state here only the equivalent definition of Sobolev spaces of periodic functions on the interval $[0,1]$, in this case we need the Fourier series expansions (see [Kre89]). For a function $\varphi \in L^2((0,1))$ we define the Fourier coefficients*

$$a_m = \int_0^1 \varphi(t) \exp^{-imt}\, dt.$$

For $k \in \mathbf{R}_+$ we denote by $H^k([0,1))$ the space of all functions $\varphi \in L^2((0,1))$ with the property

$$\sum_{m=-\infty}^{\infty} (1+m^2)^k |a_m|^2 < \infty \tag{3.7}$$

for the Fourier coefficients a_m of φ. The norm, respective the inner product in this Sobolev space are written as

$$\|\varphi\|_k = \left\{ \sum_{m=-\infty}^{\infty} (1+m^2)^k |a_m|^2 \right\}^{\frac{1}{2}},$$
$$\langle \varphi, \psi\rangle_k = \sum_{m=-\infty}^{\infty} (1+m^2)^k a_m \overline{b}_m$$

for all $\varphi, \psi \in H^k((0,1))$ with Fourier coefficients a_m, respectively b_m.

We give now some examples of Friedrichs extensions which we will use in the following chapters.

Example 3.17. *Let Ω be a bounded, smooth domain in $\mathbf{R}^m$, $m \ge 1$. Set $X_0 = L^2(\Omega)$ and let us consider the restriction of the Laplacian operator $-\triangle$ to $D(-\triangle) = C_0^\infty(\Omega)$. We consider $\mathcal{X}_1 = H_0^1(\Omega)$, where $H_0^1(\Omega)$ is the Sobolev* *space of functions defined above. We have a natural inclusion* $H_0^1(\Omega) \hookrightarrow L^2(\Omega)$ *and, from Friedrichs method there exists a self-adjoint operator* L *on* $L^2(\Omega)$ *such that*

$$\langle Lu, v\rangle_{L^2(\Omega)} = \langle u, v\rangle_1\,, \text{ for } u \in D(L), v \in H_0^1(\Omega)$$

with

$$D(L) = \left\{u \in H_0^1(\Omega) : \exists f \in L^2(\Omega) \text{ such that } \langle u, v\rangle_1 = \langle f, v\rangle_{L^2(\Omega)}\,, \forall v \in H_0^1(\Omega)\right\}.$$

With the help of Green's theorem we can rewrite the relation from the definition as

$$\langle f, v\rangle_{L^2(\Omega)} = \langle (I - \triangle)u, v\rangle_{L^2(\Omega)}$$

and it follows from general regularity results (see eg. [Wlo87]) that $L = I - \triangle$ *with the domain*

$$D(L) = \left\{u \in H_0^1(\Omega) : \triangle u \in L^2(\Omega)\right\} = H_0^1(\Omega) \cap H^2(\Omega).$$

It follows that L *is the shifted negative Laplacian with Dirichlet boundary conditions.*

Example 3.18. *Assuming again that* Ω *is a smooth bounded domain and choosing* $\mathcal{X}_1 = H^1(\Omega)$ *we can apply again the Friedrichs extension and, from regularity results for partial differential equations we obtain* $L = I - \triangle$ *with*

$$D(L) = \left\{u \in H^1(\Omega) : \exists f \in L^2(\Omega) \text{ such that } \langle u, v\rangle_1 = \langle f, v\rangle_{L^2(\Omega)}\,, \forall v \in H^1(\Omega)\right\}.$$

As $D(L) = \{u \in H^2(\Omega) : \partial_\nu u = 0 \text{ on } \partial\Omega\}$ *(see [Tay96a, Proposition 7.2]), it follows that in this case* L *corresponds to the Laplacian with Neumann boundary conditions.*

We present now some examples of self-adjoint, unbounded operators, which we will use in the Chapter 6.

Example 3.19. *Let us now consider the differential operator*

$$\begin{aligned} T(a) &: H^2(\Omega) \cap H_0^1(\Omega) \to L^2(\Omega), \\ T(a)v &= - \triangle v + av \end{aligned}$$

where $a \in L^\infty(\Omega)$*. Then* $T(a)$ *is unbounded and self-adjoint as a densely defined operator in* $L^2(\Omega)$*. We prove first that the operator is symmetric. Repeatedly* *applying the Green's theorem we have*

$$\begin{aligned}\langle T(a)u, v\rangle_{L^2(\Omega)} &= \int_\Omega (-\triangle u + au)v\, dx = \int_\Omega -\triangle uv\, dx + \int_\Omega auv\, dx \\ &= -\int_{\partial\Omega} \frac{\partial u}{\partial \nu} v\, d\sigma + \int_\Omega \bigtriangledown u \bigtriangledown v\, dx + \int_\Omega auv\, dx \\ &= -\int_\Omega u \triangle v\, dx + \int_{\partial\Omega} \frac{\partial v}{\partial \nu} u\, d\sigma + \int_\Omega auv\, dx \\ &= \int_\Omega u(-\triangle v + av)\, dx = \langle u, T(a)v\rangle_{L^2(\Omega)}\end{aligned}$$

for all $u, v \in H^2(\Omega) \cap H_0^1(\Omega)$, because, from trace theorem, $u|_{\partial\Omega} \equiv 0$ and $v|_{\partial\Omega} \equiv 0$. In order to prove that $T(a)$ is self-adjoint, we use Lemma 3.9. From classical results in partial differential equation (see eg. [Wlo87]) we know that for $a \in L^\infty(\Omega)$ and $f \in L^2(\Omega)$ there exists a unique solution $u_a \in H^2(\Omega) \cap H_0^1(\Omega)$ of the operator equation $T(a)u = f$. This means that $R(T(a)) = L^2(\Omega)$, and, as $T(a)$ is also symmetric, from (3.9) it follows that $T(a)$ is self-adjoint.

Example 3.20. *Another example of unbounded, self-adjoint operator is*

$$T(a) : H^2((0,1)) \cap H_0^1((0,1)) \to L^2((0,1)),\ T(a)u := -(au')' \tag{3.8}$$

where the parameter $a \in L^\infty((0,1))$ satisfies $a \geq \underline{a} > 0$ for some $\underline{a} \in \mathbf{R}$. As in the previous example, we check the symmetry of $T(a)$. For $u, v \in H^2((0,1)) \cap H_0^1((0,1))$ we have

$$\begin{aligned}\langle T(a)u, v\rangle_{L^2([0,1))} &= \int_0^1 -(au')'v\, dx = -(au'v)(1) + (au'v)(0) + \int_0^1 au'v'\, dx \\ &= (auv')(1) - (auv')(0) - \int_0^1 u(av')'\, dx = \langle u, T(a)v\rangle_{L^2((0,1))}.\end{aligned}$$

$T(a)$ is also surjective, as there exists a unique weak solution u_a to the operator equation $T(a)u = f$ for a given parameter a and for $f \in L^2((0,1))$, and u_a belongs to the Sobolev space $H^2((0,1))$ (see [Wlo87]). From Lemma 3.9 it follows that $T(a)$ is self-adjoint.

3.3 Hilbert scales

In this section we present a short introduction to the theory of Hilbert scales, following [EHN96]. For a more detailed presentation, see also [KP66]. It is common practice to study a variety of problems in a functional analytic setting. In partial differential equations, for example, we investigate the problems in a framework depending on the notions of space (normed, Banach, Hilbert etc) and operator. Since we need very often different series of spaces in order to express

the smoothness of the solutions, the behavior near the boundary of a domain etc., Hilbert scales are very useful for a general treatment of the problem. We will generate the spaces necessary to explore the problems with the help of operators. The interpretation of source conditions, defined with the help of functional calculus for a smoothing operator L, is an example in this sense. For some important problems they can be interpreted as classical smoothness conditions in terms of Sobolev spaces.
A natural setting to consider is a linear operator L defined between two Hilbert spaces $\mathcal{X}_1$ and $\mathcal{X}_0$. Let $\|\cdot\|_1$ and $\|\cdot\|_0$ be two norms such that

$$\|Lx\|_0 \leq c\|x\|_1$$

for all $x \in \mathcal{X}_1$. A knowledge of the set $\mathcal{M}_L$ of all pairs of Hilbert spaces $\mathcal{X}_1$ and $\mathcal{X}_0$ and the norms $\|L\|_{\mathcal{X}_1 \to \mathcal{X}_0}$ contains a fairly complete information about the operator L. Since the set $\mathcal{M}_L$ is not perspicuous, we restrict ourself to families of pairs of spaces $\mathcal{X}_0$ and $\mathcal{X}_1$, which usually depend on one or more parameters. One of the important methods of isolating such one-parameter families of spaces (which we will use in the following) is the one of the interpolation theorems. For a comprehensive treatment of this method see [KP66].
Any densely defined, unbounded, self-adjoint, strictly-positive operator L in the Hilbert space $\mathcal{X}$ is the generates a Hilbert scale. We consider the set $\mathcal{M}$, dense in $\mathcal{X}$, of all elements x for which all the powers of L are defined $\mathcal{M} = \cap_{k=0}^{\infty} D(L^k)$. $\mathcal{M}$ is dense in $\mathcal{X}$ and, by spectral theorem, L^s is well-defined for all $s \in \mathbf{R}$.

Definition 3.21. *For $x, y \in \mathcal{M}$ and $s \in \mathbf{R}$, let*

$$\langle x, y \rangle_s := \langle L^s x, L^s y \rangle,$$
$$\|x\|_s = \|L^s x\|.$$

Then the Hilbert space $\mathcal{X}_s$ is defined as the completion of $\mathcal{M}$ with respect to the norm $\|\cdot\|_s$ and $(\mathcal{X}_s)_{s \in \mathbf{R}}$ is called the ***Hilbert scale induced by*** *L.*

We state now the main properties of a Hilbert scale, for the proof see [EHN96, Proposition 8.19].

Proposition 3.22. *Let L be as above and let $(\mathcal{X}_s)_{s \in \mathbf{R}}$ be the Hilbert scale induced by L. Then the following assertions hold:*

1. *Let $-\infty < s < t < \infty$. Then the space $\mathcal{X}_t$ is densely and continuously embedded in $\mathcal{X}_s$.*

2. *Let $s, t \in \mathbf{R}$. The operator L^{t-s}, defined on $\mathcal{M}$, has a unique extension to $\mathcal{X}_t$ which is an isomorphism from $\mathcal{X}_t$ onto $\mathcal{X}_s$. This extension, again denoted by L^{t-s}, is self-adjoint and strictly positive as restriction to $\mathcal{X}_t$ in $\mathcal{X}_s$ if $t > s$. Moreover, $L^{t-s} = L^t L^{-s}$ holds for the appropriate extensions, especially $(L^s)^{-1} = L^{-s}$.*

3. *If $s \geq 0$, then $\mathcal{X}_s = D(L^s)$ and $\mathcal{X}_{-s} = (\mathcal{X}_s)'$, i.e. $\mathcal{X}_{-s}$ is the dual space of $\mathcal{X}_s$.*

4. *Let $-\infty < q < r < s < \infty$ and let $x \in \mathcal{X}_s$. Then the interpolation inequality*
$$\|v\|_r \leq \|x\|_q^{\frac{s-r}{s-q}} \|x\|_s^{\frac{r-q}{s-q}} \tag{3.9}$$
holds.

The importance of the Friedrich's extension for generating Hilbert scales is going to be shown in the following examples. For details and proofs see [Zei95, Tay96a].

Example 3.23. *The Hilbert scale $(X_s)_{s\in\mathbf{R}}$ generated by the operator L defined in Example 3.17 is going to be used in the following chapters. In the Hilbert scale $(\mathcal{X}_s)_{s\in\mathbf{R}}$ we will choose $\mathcal{X}_0 = L^2(\Omega)$, $\mathcal{X}_2 = D(L) = H_0^1(\Omega) \cap H^2(\Omega)$ and, by Remark 3.13 $\mathcal{X}_1 = D(L^{\frac{1}{2}}) = j(\mathcal{X}_1) = H_0^1(\Omega)$.*

Example 3.24. *The Hilbert scale $(\mathcal{X}_s)_{s\in\mathbf{R}}$ generated by the operator L defined in Example 3.18 has $\mathcal{X}_0 = L^2(\Omega)$, $\mathcal{X}_1 = H^1(\Omega)$ and $\mathcal{X}_2 = D(L)$. These two examples illustrates the importance of boundary conditions for Hilbert scales of function spaces. A related discussion can be found in [Neu88].*

Example 3.25. *Let $T : \mathcal{X} \to \mathcal{Y}$ be an injective, linear, bounded operator from a Hilbert space $\mathcal{X}$ into another Hilbert space $\mathcal{Y}$ with non-closed range. Then $L = (TT^*)^{-1}$ induces a Hilbert scale $(\mathcal{X}_s)_{s\in\mathbf{R}}$ with*
$$\mathcal{X}_s = D((TT^*)^{-s}) = R((TT^*)^s).$$

Remark 3.26. *As a counterexample we should mention that the usual Sobolev spaces $(H^s(\Omega))_{s\in\mathbf{R}}$ do not form a Hilbert scale if Ω is an open bounded subset of $\mathbf{R}^n$, but, for any fixed $m \in \mathbf{N}$, $(H^s(\Omega))_{0\leq s\leq m}$ is part of a Hilbert scale (see [LM72, Neu88]).*

To compare smoothness conditions formulated in terms of Hilbert scales and smoothness conditions formulated in terms of source conditions we need the following result due to Heinz ([KP66, EHN96]).

Proposition 3.27 (Inequality of Heinz)**.** *Let L and A be two densely defined unbounded self-adjoint strictly positive operators in $\mathcal{X}$ with $D(A) \subseteq D(L)$ and*
$$\|Lx\| \leq \|Ax\| \text{ for all} x \in D(A).$$
Then for all $\nu \in [0,1]$, $D(A^\nu) \subseteq D(L^\nu)$ and
$$\|L^\nu x\| \leq \|A^\nu x\| \text{ for all } x \in D(a^\nu).$$

The following result gives some equivalent conditions for the inclusion of the range of an operator in a space belonging to a Hilbert scale (details can be found in [EN05, Neu00, Egg05]).

Corollary 3.28. *Let $F : \mathcal{X} \to \mathcal{Y}$ be a linear operator and L the generating operator of the Hilbert scale $(\mathcal{X}_s)_{s\in\mathbf{R}}$ as we presented before. The following assertions are equivalent:*
1. For some $p > 0$ and $\Gamma > 0$

$$\|Fx\| \leq \Gamma\|x\|_{-p} \text{ for all } x \in \mathcal{X}$$

holds and that the extension of F to $\mathcal{X}_{-p}$ (again denoted by F) is injective.
2. It holds that

$$R(F^*) \subseteq \mathcal{X}_p \text{ and } \|F^*w\|_p \leq \Gamma\|w\| \text{ for all } w \in \mathcal{Y}.$$

If $B := FL^{-s}$ for some $s \geq -p$ and the conditions from above are fulfilled we have that

$$\begin{aligned} D((B^*B)^{\frac{-\nu}{2}}) = R((B^*B)^{\frac{\nu}{2}}) &\subseteq \mathcal{X}_{\nu(p+s)} \\ \|(B^*B)^{\frac{\nu}{2}}x\| \leq \Gamma^{\nu}\|x\|_{-\nu(p+s)} &\text{ for all } x \in \mathcal{X} \\ \|(B^*B)^{\frac{-\nu}{2}}x\| \geq \Gamma^{-\nu}\|x\|_{\nu(p+s)} &\text{ for all } x \in D((B^*B)^{\frac{-\nu}{2}}) \end{aligned}$$

for all $\nu \in [0, 1]$.
We also have equivalence between the next assertions:
3. For some $\overline{p} > 0$ and $\gamma > 0$

$$\|Fx\| \geq \gamma\|x\|_{-\overline{p}} \text{ for all } x \in \mathcal{X}.$$

4. It holds that

$$\mathcal{X}_{\overline{p}} \subseteq R(F^*) \text{ and } \|F^*w\|_{\overline{p}} \leq \gamma\|w\| \text{ for all } w \in N(F^*)^{\perp} \text{ with } F^*w \in \mathcal{X}_{\overline{p}}.$$

Under conditions $3-4$ we have that

$$\begin{aligned} \mathcal{X}_{\nu(\overline{p}+s)} \subseteq D((B^*B)^{\frac{-\nu}{2}}) &= R((B^*B)^{\frac{\nu}{2}}) \\ \|(B^*B)^{\frac{\nu}{2}}x\| \geq \gamma^{\nu}\|x\|_{-\nu(\overline{p}+s)} &\text{ for all } x \in \mathcal{X} \\ \|(B^*B)^{\frac{-\nu}{2}}x\| \leq \gamma^{-\nu}\|x\|_{\nu(\overline{p}+s)} &\text{ for all } x \in \mathcal{X}_{\nu(\overline{p}+s)} \end{aligned}$$

for B as before and for all $\nu \in [0, 1]$.

Remark 3.29. *From condition 1 in the corollary we have that*

$$R(F^*) = R((F^*F)^{\frac{1}{2}}) \subseteq \mathcal{X}_p$$

and hence it follows that

$$R((F^*F)^\mu) \subseteq \mathcal{X}_{2p\mu} \text{ for } 0 \leq \mu \leq \frac{1}{2}.$$

On the other hand, condition 3 *implies the converse inclusion*

$$\mathcal{X}_{2p\mu} \subseteq R((F^*F)^\mu) \text{ for } 0 \leq \mu \leq \frac{1}{2}.$$

The usual condition in Hilbert scale regularization is the following norm equivalence

$$\gamma\|x\|_{-p} \leq \|Fx\| \leq \Gamma\|x\|_{-p} \text{ for } x \in \mathcal{X}$$

for some $p > 0$ *and* $0 < \gamma < \Gamma < \infty$. *In this case the spaces* $\mathcal{X}_{2p\mu}$ *and* $R((F^*F)^\mu)$ *coincide for* $|\mu| \leq \frac{1}{2}$.

3.4 Regularization of linear inverse problems in Hilbert scales

In this section we review some results about a special type of regularization method, namely regularization in Hilbert scales. This method is, as mentioned in section 2.4, one way to overcome the problem of the qualification 1 of the Tikhonov regularization. Regularization in Hilbert scales was first introduced for the special case of Tikhonov regularization by Natterer (see [Nat84]) for a linear inverse problem $F(a^\dagger) = u^\dagger$. He chose the estimator a_α^δ as the solution of the minimization problem for the generalized Tikhonov functional

$$\|F(a) - Y^\delta\|_{\mathcal{Y}}^2 + \alpha\|a\|_s^2$$

over $a \in \mathcal{X}_s$, where $\{\mathcal{X}_s\}_{s\in\mathbf{R}}$ is the Hilbert scale defined in Chapter 3 and Y^δ are the noisy data with $\|Y^\delta - u^\dagger\| \leq \delta$.
Tikhonov regularization in Hilbert scales with a-priori choice of the regularization parameter proved to be order optimal in the case of the linear inverse problems. Moreover, Natterer proved that the only mistake one can make is to regularize with a norm of too small order s, higher order regularization presents no problem, even with an order bigger than the smoothness of the solution.
The theory requires that the operator F fulfills the condition

$$\lambda\|h\|_{-p} \leq \|F(h)\|_{\mathcal{Y}} \leq \Lambda\|h\|_{-p} \tag{3.10}$$

for a known $p \geq 0$, which is usually interpreted as the degree of ill-posedness. By Remark 3.29 the smoothness condition $a^\dagger \in \mathcal{X}_q$ is equivalent to the source condition $a^\dagger \in R\left((F^*F)^{\frac{q}{2p}}\right)$. From Definition 2.1 the optimal error bound is

$$\inf_R \sup_{a^\dagger\in\mathcal{X}_q} \sup_{\|\xi\|\leq 1} \|R(F(a^\dagger) + \delta\xi) - a^\dagger\|_0 = \mathcal{O}\left(\delta^{\frac{q}{p+q}}\right).$$

.

Theorem 3.30. *If F is a bounded, linear operator satisfying condition (3.10), $a^\dagger \in \mathcal{X}_q$ with $q \geq 0$ and the regularization parameter is chosen a-priori as $\alpha \sim \left(\frac{\delta}{\|u^\dagger\|_q}\right)^{\frac{2(p+s)}{p+q}}$, then the rate of convergence for the estimator a_α^δ is*

$$\|a_\alpha^\delta - a^\dagger\| = \mathcal{O}\left(\delta^{\frac{q}{p+q}}\right).$$

if $q \leq p + 2s$.

This shows that Tikhonov regularization in Hilbert scales with a-priori choice of the regularization parameter is order optimal in the case of the linear inverse problems.

We will focus now on the results obtained for linear statistical inverse problems. Linear statistical inverse problems have been studied in a Hilbert scale setting in [MP01, MR96, NP99, GP03]. We consider the noise model (2.3) with Hilbert-space process ϵ. The operator F is assumed to be compact, injective and linear, satisfying (3.10) and having a spectral decomposition

$$F = \sum_{k=1}^{\infty} \lambda_k \varphi_k \langle \psi_k, \cdot \rangle_{\mathcal{Y}}$$

where $\{\psi_k\}$, $\{\varphi_k\}$ are orthonormal bases in $\mathcal{X}$, respectively $\mathcal{Y}$ and the eigenvalues decrease like $\lambda_k \sim k^{-p}$. Moreover, we assume that L can be represented in the form

$$L = \sum_{k=1}^{\infty} l_k \psi_k \langle \psi_k, \cdot \rangle,$$

with eigenvalues of order $l_k \sim k$. Furthermore, we assume that the process ϵ can be written

$$\varepsilon = \sum_{k=1}^{\infty} \rho_k \varepsilon_k \langle \varphi_k, \cdot \rangle \varphi_k$$

where ε_k are independent, identically distributed $N(0,1)$ and $\rho_k \sim k^b$. Then the following lower bound for the minimax rate was obtained in [NP99]

$$\inf_R \sup_{a^\dagger \in \mathcal{X}_q} \sqrt{\mathbf{E}\|R(F(a^\dagger) + \sigma\epsilon) - a^\dagger\|_0^2} \geq c\sigma^{\frac{q}{q+p-b+\frac{1}{2}}}$$

for some $c > 0$. In particular, if ϵ is white noise process, the rate is

$$\inf_R \sup_{a^\dagger \in \mathcal{X}_q} \sqrt{\mathbf{E}\|R(F(a^\dagger) + \sigma\epsilon) - a^\dagger\|_0^2} \geq c\sigma^{\frac{q}{q+p+\frac{1}{2}}}.$$

The apparent difference between the deterministic and stochastic rates is explained by Nussbaum by the smoothness of degree $\frac{1}{2}$ of the Gaussian white noise, which determines the 'effective ill-posedness' of the inverse problem to be $p + \frac{1}{2}$. It follows that for the same 'ill-posedness' and 'smoothness' the two rates actually coincide. We will take advantage of this result in the section 4.3, where we study the optimality of our method.

Chapter 4

Rates of convergence for a-priori choice of regularization parameter

In this chapter we study rates of convergence for Tikhonov regularizatin in Hilbert scale for nonlinear inverse problems with stochastic noise. Starting from the method introduced in [BHM04] and discussed in section 2.5 we introduce an estimator $\widehat{a}$ for the unknown function $a^\dagger$ and we study rates of convergence for expected squared error and optimality of the method. To achieve these goals we use Hilbert scales as introduced in section 3.4. Our analysis in section 4.1, and in particular the second part of the proof of our general convergence theorem are based on the work of Neubauer [Neu92] on nonlinear Tikhonov regularization with deterministic noise.
The plan of this chapter is as follows: In the following section we prove a general result on the rates of convergence of nonlinear Tikhonov regularization in Hilbert scales for random noise with a-priori choice of the regularization parameter. The optimality of the overall two-step method to estimate $a^\dagger$ from data described by (2.3) is discussed in section 4.3.

4.1 Review of convergence results for deterministic setting

We assume now the same deterministic noise model as in section 2.2, Hilbert scales introduced in section 3.4 and we assume that the operator F is nonlinear. Following [Neu92] we define the estimator a_α^δ of $a^\dagger$ by

$$a_\alpha^\delta := \operatorname{argmin}_{a\in D(F)\cap(a_0+\mathcal{X}_s)} \left(\|F(a)-Y^\delta\|_{\mathcal{Y}}^2 + \alpha\|a-a_0\|_s^2\right) \tag{4.1}$$

where $s \geq 0$ and $a_0 \in \mathcal{X}$ an initial guess. By regularization in Hilbert scales the finite qualification of Tikhonov regularization can be overcome, i.e. the rate of convergence is not bounded by $\|a_\alpha^\delta - a^\dagger\| = O(\delta^{2/3})$, but given sufficient smoothness of the solution, the exponent of δ may be arbitrarily close to 1. Compared to simple Tikhonov regularization, regularization in Hilbert scales for nonlinear inverse problems has not only the advantage of overcoming the saturation but also needs less restrictive conditions on $a^\dagger$ since we got rid of the smallness assumption on the norm of the source element v (see (4)). If we apply the theory for Tikhonov regularization to our estimator a_α^δ, we obtain convergence results for s-norm of a_α^δ, but we are interested in the rates of convergence in the original norm and such a result was obtained by Neubauer (see [Neu92]) for a-priori choice of the regularization parameter. We present here this result (see also [EHN96]).

Assumptions 4.1.

1. *There exists a unique a_0-minimum-norm solution $a^\dagger$ in $\mathcal{X}_s$, i.e. $a^\dagger \in D(F) \cap \mathcal{X}_s$, $F(a^\dagger) = u^\dagger$ and $\|a^\dagger - a_0\|_{\mathcal{X}} = \min\left\{\|a - a_0\|_s | F(a) = u^\dagger\right\}$. $D(F)$ is convex, F is nonlinear, continuous and Fréchet-differentiable on $\mathcal{X}$ and weakly (sequentially) closed on $\mathcal{X}_s$ for some $s \geq 0$.*

2. *There exist $\epsilon > 0$ and $C_L > 0$ such that $\|F'(a^\dagger) - F'(a)\|_{\mathcal{Y}\to\mathcal{X}} \leq C_L \|a^\dagger - a\|_{\mathcal{X}}$ for all $a \in D(F) \cap B_\epsilon(a^\dagger)$.*

3. *$\|F'(a^\dagger)h\|_{\mathcal{Y}} \sim \|h\|_{-p}$ for all $h \in \mathcal{X}$ for some known $p > 0$.*

Theorem 4.2. *Let $Y^\delta \in \mathcal{Y}$ be such that $\|Y^\delta - u^\dagger\|_{\mathcal{Y}} \leq \delta$ and let Assumptions 4.1 and the smoothness condition*

$$a^\dagger - a_0 \in \mathcal{X}_q, \text{ for some } q \in [s, p + 2s], s \geq p$$

hold. Then for the choice $\alpha \sim \delta^{\frac{2(p+s)}{p+q}}$ we obtain

$$\|a_\alpha^\delta - a^\dagger\|_{\mathcal{X}} = \mathcal{O}\left(\delta^{\frac{q}{p+q}}\right).$$

Remark 4.3. *The rate of convergence in the nonlinear case, as in the linear inverse problems, does not depend on the norm index s which we use in the regularization term. In the linear case the same rates of convergence were obtained if the parameter s is bigger or smaller than q, under the only condition that $s \geq \frac{q-p}{2}$. For a nonlinear operator, order optimal rates of convergence were obtained only in the case of low-order regularization, i.e. for $s \leq q$. It is still an open problem whether order optimal rates can be obtained for $s > q$, but it seems that much more restricitve assumptions on the degree of nonlinearity of F will be necessary.*

As usual, the a-priori choice of the regularization parameter is not realizable, as the smoothness of the solution is not known. For the choice $\alpha = \mathcal{O}(\delta^2)$ we obtain, under stronger assumptions, the order optimal rates of convergence (see

[EHN96]). This regularization parameter choice does not require the knowledge of the smoothness condition. Convergence rates results for Tikhonov regularization in Hilbert scales with a-posteriori choice of the regularization parameter for nonlinear inverse problems were not studied until now. Other regularization methods for nonlinear inverse problems in Hilbert scales with deterministic noise have been studied in [EN05, Neu00, Tau96]. As we mentioned before, nonlinear statistical inverse problems in Hilbert scales have not been studied until now. In the next section we are going to obtain rates of convergence for Tikhonov regularization in Hilbert scales for inverse problems with stochastic noise.

4.2 Rates of convergence in stochastic setting

In a similar way as before we define the statistical estimator $\widehat{a}$ of $a^\dagger$ by

$$\widehat{a} := \operatorname{argmin}_{a \in D(F) \cap (a_0 + \mathcal{X}_s)} \left(\|F(a) - \widehat{u}\|_{\mathcal{Y}}^2 + \alpha \|a - a_0\|_s^2 \right) \tag{4.2}$$

where $s \geq 0$ and $a_0 \in \mathcal{X}$ an initial guess. To bound the error $\mathbf{E}(\|\widehat{a} - a^\dagger\|_{\mathcal{X}}^2)$ we need the following assumptions:

Assumptions 4.4.

A) *(assumptions on F) If $F(a) = F(a^\dagger)$ for some $a \in D(F) \cap (a_0 + \mathcal{X}_s)$, then $a = a^\dagger$. Moreover, $D(F)$ is convex, $F : D(F) \cap (a_0 + \mathcal{X}_s) \to \mathcal{Y}$ is weakly sequentially closed, and $F : D(F) \subset \mathcal{X} \to \mathcal{Y}$ has a Fréchet derivative $F' : D(F) \to L(\mathcal{X}, \mathcal{Y})$.*

B) *(smoothing properties of F') There exist constants $p \in [0, s]$ and $\lambda, \Lambda > 0$ such that for all $h \in \mathcal{X}$*

$$\lambda \|h\|_{-p} \leq \|F'(a^\dagger) h\|_{\mathcal{Y}} \leq \Lambda \|h\|_{-p}. \tag{4.3}$$

C) *(Lipschitz continuity of F') There exists a constant $C_L > 0$ such that*

$$\|F'(a) - F'(a^\dagger)\|_{\mathcal{Y} \leftarrow \mathcal{X}_{-p}} \leq C_L \|a - a^\dagger\|_{\mathcal{X}} \leq \frac{\lambda^2}{2\Lambda} \tag{4.4}$$

for all $a \in D(F) \cap (a_0 + \mathcal{X}_s)$.

We notice that if $\widehat{u}$ is stochastic then the norm $\|\cdot\|_{\mathcal{Y} \leftarrow \mathcal{X}}$ in Assumption 2 is replaced by $\|\cdot\|_{\mathcal{Y} \leftarrow \mathcal{X}_{-p}}$ in (4.4). This stronger condition will be necessary to control the Taylor remainder of F in the proof of Theorem 4.6. A condition similar to (4.4) has been used in [Neu00] (in fact, condition (iv) in [Neu00, Assumption 2.1] with $\beta = 1$ and $b = p$ is equivalent to the first inequality in (4.4)). We state now a result which is going to be very useful in the following.

Lemma 4.5. *If the inequality*

$$c^r \leq e + dc^t \tag{4.5}$$

holds for some $0 \leq t < r$ *and* $c, d, e > 0$ *then*

$$c^r = \mathcal{O}\left(e + d^{\frac{r}{r-t}}\right).$$

Proof. To prove our implication we need Young inequality

$$ab \leq \frac{a^\tau}{\tau} + \frac{b^\mu}{\mu} \tag{4.6}$$

for all $1 < \tau, \mu < \infty$, $\frac{1}{\tau} + \frac{1}{\mu} = 1$. We apply Young inequality for $a = d$, $b = c^t$, $\tau = \frac{r}{r-t}$, $\mu = \frac{r}{t}$. It follows that

$$c^r \leq e + \frac{d^{\frac{r}{r-t}}}{\frac{r}{r-t}} + \frac{c^r}{\frac{r}{t}}.$$

Then we have

$$(1 - \frac{t}{r})c^r \leq e + \frac{r-t}{r} d^{\frac{r}{r-t}}$$

and, since $0 \leq t < r$, this implies our conclusion. □

Theorem 4.6. *Let* $a^\dagger \in D(F)$ *be the solution of operator equation (1.1), and let* $\widehat{u}$ *be an estimator of* u *satisfying (1.5). If the Assumptions 4.4–4.4 hold true and if*

$$a^\dagger - a_0 \in \mathcal{X}_q \qquad \textit{for some } q \in [s, 2s+p] \tag{4.7}$$

then, for the a-priori choice of the regularization parameter $\alpha \sim \beta^{\frac{2(p+s)}{p+q}}$, *we obtain*

$$\sqrt{\mathbf{E}\|\widehat{a} - a^\dagger\|^2_{\mathcal{X}}} = \mathcal{O}\left(\beta^{\frac{q}{p+q}}\right), \qquad \beta \to 0. \tag{4.8}$$

Proof. By the definition (4.2) of $\widehat{a}$ as a solution to the minimization problem we have

$$\|F(\widehat{a}) - \widehat{u}\|^2_{\mathcal{Y}} + \alpha\|\widehat{a} - a_0\|^2_s \leq \|u^\dagger - \widehat{u}\|^2_{\mathcal{Y}} + \alpha\|a^\dagger - a_0\|^2_s$$

and hence

$$\begin{aligned} & \|F(\widehat{a}) - \widehat{u}\|^2_{\mathcal{Y}} + \alpha\|\widehat{a} - a^\dagger\|^2_s \\ \leq \;& \|u^\dagger - \widehat{u}\|^2_{\mathcal{Y}} + \alpha\left(\|a^\dagger - a_0\|^2_s - \|\widehat{a} - a_0\|^2_s + \|\widehat{a} - a^\dagger\|^2_s\right) \\ = \;& \|u^\dagger - \widehat{u}\|^2_{\mathcal{Y}} + 2\alpha\left\langle a^\dagger - a_0, a^\dagger - \widehat{a}\right\rangle_s. \end{aligned}$$

Using the hypothesis $a^\dagger - a_0 \in \mathcal{X}_q$ we obtain

$$\|F(\widehat{a}) - \widehat{u}\|^2_{\mathcal{Y}} + \alpha\|\widehat{a} - a^\dagger\|^2_s \leq \|u^\dagger - \widehat{u}\|^2_{\mathcal{Y}} + 2\alpha\|a^\dagger - \widehat{a}\|_{2s-q}\|a^\dagger - a_0\|_q. \tag{4.9}$$

Introducing the Taylor remainder $e_{\text{tay}} := F(\widehat{a}) - F(a^\dagger) - F'(a^\dagger)(\widehat{a} - a^\dagger)$ we obtain the inequality

$$\begin{aligned}
&\|F(\widehat{a}) - \widehat{u}\|_{\mathcal{Y}}^2 = \|u^\dagger - \widehat{u} + e_{\text{tay}} + F'(a^\dagger)(\widehat{a} - a^\dagger)\|_{\mathcal{Y}}^2 \\
&= \|u^\dagger - \widehat{u} + e_{\text{tay}}\|_{\mathcal{Y}}^2 + \|F'(a^\dagger)(\widehat{a} - a^\dagger)\|_{\mathcal{Y}}^2 + 2\left\langle F'(a^\dagger)(\widehat{a} - a^\dagger), u^\dagger - \widehat{u} + e_{\text{tay}}\right\rangle \\
&\geq \lambda^2 \|\widehat{a} - a^\dagger\|_{-p}^2 - 2\Lambda\|\widehat{a} - a^\dagger\|_{-p}\left(\|u^\dagger - \widehat{u}\|_{\mathcal{Y}} + \|e_{\text{tay}}\|_{\mathcal{Y}}\right).
\end{aligned}$$

Plugging this into (4.9) yields

$$\begin{aligned}
\lambda^2\|\widehat{a} - a^\dagger\|_{-p}^2 + \alpha\|\widehat{a} - a^\dagger\|_s^2 &\leq \|u^\dagger - \widehat{u}\|_{\mathcal{Y}}^2 + 2\alpha\|a^\dagger - \widehat{a}\|_{2s-q}\|a^\dagger - a_0\|_q \\
&+2\Lambda\|\widehat{a} - a^\dagger\|_{-p}\|e_{\text{tay}}\|_{\mathcal{Y}} + 2\Lambda\|\widehat{a} - a^\dagger\|_{-p}\|u^\dagger - \widehat{u}\|_{\mathcal{Y}}.
\end{aligned}$$

By the interpolation inequality (3.9) for $t = -p$, $r = 2s - q$ and $s = s$ we have

$$\|\widehat{a} - a^\dagger\|_{2s-q} \leq \|\widehat{a} - a^\dagger\|_{-p}^{\frac{-s+q}{s+p}}\|\widehat{a} - a^\dagger\|_s^{\frac{2s-q+p}{s+p}}. \tag{4.10}$$

Replacing this term in our estimate and taking the mean in the inequality we get

$$\begin{aligned}
&\lambda^2\mathbf{E}\|\widehat{a} - a^\dagger\|_{-p}^2 + \alpha\mathbf{E}\|\widehat{a} - a^\dagger\|_s^2 \qquad (4.11)\\
\leq\ & \mathbf{E}\|u^\dagger - \widehat{u}\|_{\mathcal{Y}}^2 + 2\alpha\|a^\dagger - a_0\|_q\mathbf{E}\left(\|\widehat{a} - a^\dagger\|_{-p}^{\frac{-s+q}{s+p}}\|\widehat{a} - a^\dagger\|_s^{\frac{2s-q+p}{s+p}}\right) \\
&+2\Lambda\mathbf{E}\left(\|\widehat{a} - a^\dagger\|_{-p}\|e_{\text{tay}}\|_{\mathcal{Y}}\right) + 2\Lambda\mathbf{E}\left(\|\widehat{a} - a^\dagger\|_{-p}\|u^\dagger - \widehat{u}\|_{\mathcal{Y}}\right).
\end{aligned}$$

Using the Cauchy-Schwarz inequality and Jensen's inequality we obtain

$$\begin{aligned}
\mathbf{E}\left(\|\widehat{a} - a^\dagger\|_{-p}^{\frac{-s+q}{s+p}}\|\widehat{a} - a^\dagger\|_s^{\frac{2s-q+p}{s+p}}\right) &\leq \mathbf{E}^{\frac{1}{2}}\left(\|\widehat{a} - a^\dagger\|_{-p}^{2\frac{-s+q}{s+p}}\right)\mathbf{E}^{\frac{1}{2}}\left(\|\widehat{a} - a^\dagger\|_s^{2\frac{2s-q+p}{s+p}}\right) \\
&\leq \mathbf{E}^{\frac{1}{2}\frac{-s+q}{s+p}}\left(\|\widehat{a} - a^\dagger\|_{-p}^2\right)\mathbf{E}^{\frac{1}{2}\frac{2s-q+p}{s+p}}\left(\|\widehat{a} - a^\dagger\|_s^2\right)
\end{aligned}$$

since $0 \leq \frac{-s+q}{s+p} \leq 1$ and $0 \leq \frac{2s-q+p}{s+p} \leq 1$ for $s \leq q \leq 2s + p$.
Next we are going to show that the term involving the Taylor remainder e_{tay} in (4.11) is dominated by the term on the left hand side for small β:

$$2\Lambda\mathbf{E}\left(\|\widehat{a} - a^\dagger\|_{-p}\|e_{\text{tay}}\|_{\mathcal{Y}}\right) \leq \frac{\lambda^2}{2}\mathbf{E}\|\widehat{a} - a^\dagger\|_{-p}^2 \tag{4.12}$$

Using Assumption 4.4, the Taylor remainder e_{tay} can be estimated by

$$\begin{aligned}
\|e_{\text{tay}}\|_{\mathcal{Y}} &= \|F\left(\widehat{a}\right) - F(a^\dagger) - F'(a^\dagger)\left(\widehat{a} - a^\dagger\right)\|_{\mathcal{Y}} \\
&= \left\|\int_0^1 \left\{F'\left(a^\dagger + t\left(\widehat{a} - a^\dagger\right)\right) - F'(a^\dagger)\right\}\left(\widehat{a} - a^\dagger\right)\,dt\right\|_{\mathcal{Y}} \\
&\leq \int_0^1 \|F'\left(a^\dagger + t\left(\widehat{a} - a^\dagger\right)\right) - F'(a^\dagger)\|_{\mathcal{Y}\leftarrow\mathcal{X}_{-p}}\|\widehat{a} - a^\dagger\|_{-p}\,dt \\
&\leq \int_0^1 C_L t\|\widehat{a} - a^\dagger\|_0\,\|\widehat{a} - a^\dagger\|_{-p}\,dt \leq \frac{C_L}{2}\|\widehat{a} - a^\dagger\|_0\,\|\widehat{a} - a^\dagger\|_{-p},
\end{aligned}$$

which implies (4.12). Altogether, we arrive at the estimate

$$\begin{aligned}
&\mathbf{E}\|\widehat{a}-a^\dagger\|_{-p}^2+\alpha\mathbf{E}\|\widehat{a}-a^\dagger\|_s^2\\
=\;&\mathcal{O}\left(\beta^2+\alpha\mathbf{E}^{\frac{1}{2}\frac{-s+q}{s+p}}\left(\|\widehat{a}-a^\dagger\|_{-p}^2\right)\mathbf{E}^{\frac{1}{2}\frac{2s-q+p}{s+p}}\left(\|\widehat{a}-a^\dagger\|_s^2\right)+\beta\mathbf{E}^{\frac{1}{2}}\left(\|\widehat{a}-a^\dagger\|_{-p}^2\right)\right).
\end{aligned}$$

using also assumption (1.5). In the following, we will make repeated use of the Lemma (4.5) for $c=\mathbf{E}^{\frac{1}{2}}(\|\widehat{a}-a^\dagger\|_{-p}^2)$ and $r=2$. First we take $t=1$, $d=\beta$ and $e=\beta^2+\alpha\mathbf{E}^{\frac{1}{2}\frac{-s+q}{s+p}}\left(\|\widehat{a}-a^\dagger\|_{-p}^2\right)\mathbf{E}^{\frac{1}{2}\frac{2s-q+p}{s+p}}\left(\|\widehat{a}-a^\dagger\|_s^2\right)$ and we obtain

$$\mathbf{E}\|\widehat{a}-a^\dagger\|_{-p}^2=\mathcal{O}\left(\beta^2+\alpha\mathbf{E}^{\frac{1}{2}\frac{-s+q}{s+p}}\left(\|\widehat{a}-a^\dagger\|_{-p}^2\right)\mathbf{E}^{\frac{1}{2}\frac{2s-q+p}{s+p}}\left(\|\widehat{a}-a^\dagger\|_s^2\right)\right)$$

then we choose $t=\frac{q-s}{p+s}$, $d=\alpha\mathbf{E}^{\frac{1}{2}\frac{2s-q+p}{s+p}}\left(\|\widehat{a}-a^\dagger\|_s^2\right)$ and $e=\beta^2$ and we get

$$\mathbf{E}\|\widehat{a}-a^\dagger\|_{-p}^2=\mathcal{O}\left(\beta^2+\alpha^{\frac{2(s+p)}{3s+2p-q}}\mathbf{E}^{\frac{2s-q+p}{3s+2p-q}}\left(\|\widehat{a}-a^\dagger\|_s^2\right)\right).$$

Replacing the term that contains $\mathbf{E}\|\widehat{a}-a^\dagger\|_{-p}^2$ on the right hand side and using the inequality $(x+y)^r\le x^r+y^r$ for $0\le r\le 1$ we obtain

$$\begin{aligned}
\mathbf{E}\|\widehat{a}-a^\dagger\|_s^2=\mathcal{O}\Big(&\alpha^{-1}\beta^2+\beta\alpha^{\frac{q-2s-p}{3s+2p-q}}\mathbf{E}^{\frac{p}{2}\frac{2s-q+p}{3s+2p-q}}\left(\|\widehat{a}-a^\dagger\|_s^2\right)\\
&+\beta^{\frac{-s+q}{s+p}}\mathbf{E}^{\frac{1}{2}\frac{2s-q+p}{s+p}}\left(\|\widehat{a}-a^\dagger\|_s^2\right)+\alpha^{\frac{-s+q}{3s+2p-q}}\mathbf{E}^{\frac{2s-q+p}{3s+2p-q}}\left(\|\widehat{a}-a^\dagger\|_s^2\right)\Big).
\end{aligned}$$

Applying Lemma (4.5) repeatedly for $c=\mathbf{E}\|\widehat{a}-a^\dagger\|_s^2$, $r=1$ and $t=\frac{2s-q+p}{2(3s+2p-q)}$, $t=\frac{1}{2}\frac{2s-q+p}{s+p}$ respectively $t=\frac{2s-q+p}{3s+2p-q}$ we obtain

$$\mathbf{E}\|\widehat{a}-a^\dagger\|_s^2=\mathcal{O}\left(\alpha^{-1}\beta^2+\beta^{\frac{2(3s+2p-q)}{4s+3p-q}}\alpha^{\frac{2(q-2s-p)}{4s+3p-q}}+\beta^{\frac{2(q-s)}{q+p}}\right)=\mathcal{O}\left(\beta^{2\frac{q-s}{p+q}}\right).$$

As $\alpha\sim\beta^{\frac{2(p+s)}{p+q}}$ it follows that

$$\begin{aligned}
\mathbf{E}\|\widehat{a}-a^\dagger\|_{-p}^2&=\mathcal{O}\left(\beta^2+\alpha^{\frac{2(s+p)}{3s+2p-q}}\mathbf{E}^{\frac{2s-q+p}{3s+2p-q}}\left(\|\widehat{a}-a^\dagger\|_s^2\right)\right)\\
&=\mathcal{O}\left(\beta^2+\beta^{4\frac{(p+s)^2}{(p+q)(3s+2p-q)}+2\frac{2s-q+p}{3s+2p-q}\frac{q-s}{p+q}}\right)=\mathcal{O}\left(\beta^2\right).
\end{aligned}$$

Taking the mean in the squared interpolation inequality (3.9) and using Jensen's inequality we get

$$\begin{aligned}
\mathbf{E}\left(\|\widehat{a}-a^\dagger\|_0^2\right)&\le\mathbf{E}\left(\|\widehat{a}-a^\dagger\|_{-p}^{\frac{2s}{s+p}}\|\widehat{a}-a^\dagger\|_s^{\frac{2p}{s+p}}\right)\\
&\le\mathbf{E}\left(\|\widehat{a}-a^\dagger\|_{-p}^2\right)^{\frac{s}{s+p}}\mathbf{E}\left(\|\widehat{a}-a^\dagger\|_s^2\right)^{\frac{p}{s+p}}\\
&=\mathcal{O}\left(\beta^{\frac{2s}{p+s}}\beta^{2\frac{q-s}{q+p}\frac{p}{s+p}}\right)=\mathcal{O}\left(\beta^{\frac{2q}{q+p}}\right).
\end{aligned}$$

$\square$

Remark 4.7. *In some cases the rates of convergence with respect to other norms in the Hilbert scale are also of interest. Introducing $r \in [-p, s]$ as an additional parameter, a straightforward modification of the very last step of the previous proof yields the estimate*

$$\sqrt{\mathbf{E}\|\widehat{a} - a^\dagger\|_r^2} = \mathcal{O}\left(\beta^{\frac{q-r}{p+q}}\right), \qquad \beta \to 0. \tag{4.13}$$

4.3 Optimality

In the following we show that our two-step method to estimate $a^\dagger$ from noisy data described by the noise model (2.9) for problem (1.1) is capable of achieving the optimal rates provided that the direct regression problem in the first step is solved in an optimal way.
For this end we consider a situation where lower bounds on the expected squared error are known. Let $F : \mathcal{X} \to \mathcal{Y}$ be a linear, compact injective operator with polynomially decaying singular values. More precisely, we assume that the singular values $\sigma_j(F)$ decay like

$$\sigma_j(F) \sim j^{-p/d}, \qquad j \in \mathbf{N}$$

for some $p, d > 0$, i.e. there exists a constant $c > 0$ such that $j^{-p/d}/c \leq \sigma_j(F) \leq cj^{-p/d}$ for all $j \in \mathbf{N}$. (Later in our applications where F acts in Sobolev scales, d will be the space dimension and p the degree of ill-posedness as in (4.3).) Consider the Hilbert scale $(\mathcal{X}_s)_{s\in\mathbf{R}}$ generated by the self-adjoint operator $L := (F^*F)^{-1/2p}$ defined on the dense subspace $D(L) := (F^*F)^{1/2p}(\mathcal{X})$. Then the eigenvalues of L behave like

$$\lambda_j(L) \sim j^{1/d}.$$

The asymptotic behavior of the minimax rates for $d = 1$ was discussed in section 3.4. For a general d, we can consider the Hilbert scale $\left(\tilde{X}_s\right)_{s\in\mathbf{R}}$ generated by the operator L^d, whose eigenvalues behave as

$$\lambda_j(L^d) \sim j.$$

For this choice of Hilbert scale the ill-posedness of our problem is equal to $\frac{p}{d}$ and the smoothness assumption $a^\dagger \in \mathcal{X}_q$ is equivalent to $a^\dagger \in \tilde{\mathcal{X}}_{\frac{q}{d}}$. Applying the results from section 3.4 for a white noise model (2.9) with $u^\dagger = Fa^\dagger$ under the smoothness assumption $\|a^\dagger\|_q \leq 1$ for the Hilbert scale $\tilde{\mathcal{X}}_s$ we obtain a lower bound on the expected squared error of an estimator $\widehat{a}$ of $a^\dagger$

$$\inf_R \sup_{\|a^\dagger\|_q \leq 1} \sqrt{\mathbf{E}\|R(\mathcal{Y}) - a^\dagger\|_{\mathcal{X}}^2} \geq c\sigma^{\frac{q}{q+p+d/2}} \tag{4.14}$$

for some $c > 0$. To show that this lower bound is achieved by our two-step method, we first study the direct regression problem to estimate $u^\dagger$ from $\mathcal{Y}$. Let $\{(v_j, u_j, \sigma_j(F)) : j \in \mathbf{N}\}$ denote a singular system of F,

$$Fa = \sum_{j=1}^{\infty} \sigma_j(F) \langle a, v_j \rangle_{\mathcal{X}} u_j$$

for $a \in \mathcal{X}$. For theoretical purposes we may assume that $F(\mathcal{X})$ is dense in $\mathcal{Y}$ (otherwise we can use the orthogonal projection onto $\overline{F(\mathcal{X})}$). Then $\{u_j : j \in \mathbf{N}\}$ is a complete orthonormal system in $\mathcal{Y}$. The assumption that $a^\dagger \in \mathcal{X}_q$ and $\|a^\dagger\|_q \leq 1$ is equivalent to the fact that $w := L^q a^\dagger$ is well-defined and $\|w\|_{\mathcal{X}} \leq 1$. The Fourier coefficients of $u^\dagger$ satisfy

$$|\langle u^\dagger, u_j \rangle_{\mathcal{Y}}| = |\langle F L^{-q} w, u_j \rangle_{\mathcal{Y}}| = |\langle w, L^{-q} F^* u_j \rangle_{\mathcal{X}}| \sim j^{-(q+p)/d} |\langle w, v_j \rangle_{\mathcal{X}}|.$$

Therefore, by Pinskers Theorem (presented shortly in (2.10)) an optimal estimator $\widehat{u}$ satisfies

$$\sqrt{\mathbf{E}\|\widehat{u} - u^\dagger\|_{\mathcal{Y}}^2} \leq \delta \qquad \text{with} \qquad \delta \sim \sigma^{\frac{p+q}{p+q+d/2}}. \tag{4.15}$$

In a second step we can compute the estimator $\widehat{a}$ defined in (4.2) with the natural choice $a_0 = 0$. Since

$$\|Fa\|_{\mathcal{Y}}^2 = (a, F^*Fa)_{\mathcal{X}} = \|(F^*F)^{1/2} a\|_{\mathcal{X}}^2 = \|L^{-p} a\|_{\mathcal{X}}^2 = \|a\|_{-p}^2$$

for all $a \in \mathcal{X}$, Assumption 4.4 is satisfied. Moreover, Assumptions 4.4 and 4.4 are trivially satisfied with $C_L = 0$. Therefore, Theorem 4.6 yields

$$\sqrt{\mathbf{E}\|\widehat{a} - a^\dagger\|_{\mathcal{X}}^2} = \mathcal{O}\left(\delta^{\frac{q}{p+q}}\right) = \mathcal{O}\left(\sigma^{\frac{q}{p+q+d/2}}\right).$$

This coincides with the lower bound (4.14). Since the two-step procedure described above yields an order-optimal error bound, in particular the error bound for the second step in Theorem 4.6 has to be of optimal order under the given assumptions.

Remark 4.8. *It seems that for nonlinear problems additional assumptions on F are required to guarantee that the direct regression problem can be solved with the accuracy (4.15). We refrain from discussing this problem in the general functional analytic setting, but show for the problems considered in Chapter 6 that this accuracy can be achieved.*

Chapter 5

Lepskii choice of the regularization parameter

We present in this chapter results regarding Lepskii choice of the regularization parameter for nonlinear deterministic and statistical inverse problems. The framework is going to be similar to the one in the previous chapter dedicated to a-priori choice of the regularization parameter. We saw in Chapter 4 that the a-priori choice of the regularization parameter which yields order-optimal rates of convergence requires the knowledge of the noise level δ and of the smoothness of the solution q. As in practice this smoothness information is not available, a-posteriori rules are necessary which choose α from quantities that arise during calculations. Morozov's discrepancy principle was generalized for non-linear ill-posed problems in [KS85, TLY98], but this method implies solving the equation

$$\|F(a_\alpha^\delta) - Y^\delta\| = \delta$$

which is also nonlinear and difficult to solve. Order optimal rates of convergence for Tikhonov regularization of nonlinear inverse problems were obtained, for a-posteriori choice of the regularization parameter, in [SEK93, TJ03, LPR07].
We will focus on the Lepskii principle, which is the a-posteriori method which we are going to apply. Lepskii developed this rule of choosing the regularization parameter in the statistical context, as an adaptive method of estimation of a value $S(t_0)$ for a function S belonging to $\Sigma(\beta, L)$, where

$$\begin{aligned}\Sigma(\beta, L) = \{&S : S\ m\text{-fold continuously differentiable on the segment } [0,1],\\ &|S^{(m)}(t_1) - S^{(m)}(t_2)| \leq L|t_1 - t_2|^\alpha, \forall t_1, t_2\}\end{aligned}$$

where m is a non-negative integer, $\alpha \in (0, 1]$, $\beta = m + \alpha$ and $L > 0$ is a constant (see [Lep90]).
The same principle of bounding the best possible accuracy by a function which is non-increasing with respect to α-values was used by Mathé and Pereverzev to obtain order-optimal estimators in variable Hilbert scales (see [MP03]). Afterwards

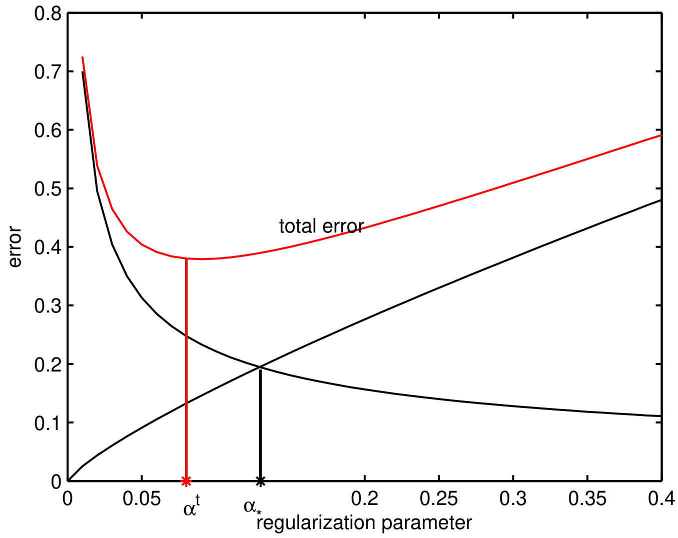

Figure 5.1: Total error, the approximation error and perturbation error with respect to the regularization parameter

this principle was applied by different authors for deterministic inverse problems [LPR07, MP03, BH05].

5.1 Lepskii's balancing principle in an abstract setting

Let $\{a_1, a_2, \ldots, a_m\}$ be a finite set of elements in some metric space (M, d) and $\Psi : \{1, \ldots, m\} \to \mathbf{R}_+$ be a non-increasing function. We define

$$\bar{i} = \max\{i \leq m, d(a_i, a_j) \leq 2\Psi(j) \text{ for all } j \leq i\}.$$

We start with the smallest value 1 in order to determine $\bar{i}$. Hence, the underlying principle is essentially based on the order of the finite set $\{1, \ldots, m\}$, cf. [Mat06]. In our application we are going to use another approach which involves the notion of admissible functions, developed in [MP06]. Usually the total error can be bounded by the sum between an increasing function Φ and a non-increasing one Ψ.

Definition 5.1. *A non-decreasing function $\Phi : \{1, \ldots, m\} \to \mathbf{R}_+$ is said to be* ***admissible*** *for $a^\dagger$, if $\Phi(1) \leq \Psi(1)$ and*

$$d(a^\dagger, a_j) \leq \frac{1}{2}(\Phi(j) + \Psi(j)), j = 1, \ldots, m. \tag{5.1}$$

Admissible functions arise from the decomposition of the total error into the approximation error and perturbation error (see Figure 5.1). The choice $\alpha = \alpha_{\bar{i}}$ with

$$\bar{i} = \max\left\{i \leq m, d(a_i, a_j) \leq 2\Psi(j) \text{ for all } j \leq i\right\}.$$

has the following interpretation (see [Mat06]).

Lemma 5.2. *Under the previous assumptions for Ψ and for*

$$i_* = \max\left\{j : \textit{ there exists admiss. } \Phi \textit{ for which } \Phi(j) \leq \Psi(j)\right\}$$

it holds

$$i_* \leq \bar{i}$$

and

$$d(a^\dagger, a_{\bar{i}}) \leq 3\Psi(i_*).$$

Proof. For any $j = 1, 2, \ldots$ such that $j \leq i_*$, we have

$$\begin{aligned}
\|a_j - a_{i_*}\| &\leq \|a_j - a^\dagger\| + \|a_{i_*} - a^\dagger\| \\
&\leq \frac{1}{2}(\Phi(j) + \Psi(j)) + \frac{1}{2}(\Phi(i_*) + \Psi(i_*)) \\
&\leq 2\Psi(j).
\end{aligned}$$

From the definition of $\bar{i}$ it follows that $i_* \leq \bar{i}$ and we can write

$$\begin{aligned}
\|a_{\bar{i}} - a^\dagger\| &\leq \|a_{\bar{i}} - a_{i_*}\| + \|a_{i_*} - a^\dagger\| \\
&\leq 2\Psi(\bar{i}) + \frac{1}{2}(\Psi(i_*) + \Phi(i_*)) \\
&\leq 2\Psi(\bar{i}) + \Psi(i_*) \\
&\leq 3\Psi(i_*).
\end{aligned}$$

□

It follows that $a^\dagger$ belongs to the ball of radius $6\Psi(i_*)$ centered in $a_{\bar{i}}$. The interpretation of $6\Psi(i_*)$ follows from the deterministic oracle inequality. This means that for the chosen regularization parameter $\min \|a_{\bar{i}} - a^\dagger\|$ attains the ideal risk up to a constant.

Corollary 5.3. *Assume that the assumptions of Lemma 5.2 hold and there exists $D < \infty$ such that the function Ψ obeys $\Psi(j) < D\Psi(j+1)$. Then we have*

$$d(a^\dagger, a_{\bar{i}}) \leq 6D \min\left\{\Psi(j) + \Phi(j), j = 1, \ldots, m, \Phi \textit{ admiss.}\right\}.$$

Proof. Let Φ be a any admissible function and let us introduce a new index

$$\tilde{i} = \operatorname{argmin} \Psi(j) + \Phi(j), j = 1, 2, \ldots, m.$$

The assertion of the corollary is an immediate consequence of $\Psi(i_*) \leq D(Psi(\tilde{i}) + \Phi(\tilde{i}))$. This is evident, because either $i_* \geq \tilde{i}$, in which case $\Psi(i_*) \leq \Psi(\tilde{i}) \leq \Psi(\tilde{i}) + \Phi(\tilde{i})$ or $i_* < i_* + 1 \leq \tilde{i}$. But in this case, by the definition of i_* it holds true $\Psi(i_* + 1) \leq \Phi(i_* + 1)$, thus

$$\Psi(i_*) \leq D\Psi(i_* + 1) \leq D\Phi(i_* + 1) \leq D\Phi(\tilde{i}),$$

from which the estimate follows. □

The interpretation is clear now: by choosing $\bar{i}$ we obtain, up to a constant, the best possible error bound from (5.1). This justifies why the Lepskii regularization parameter choice is seen as a balancing principle which tries to balance the known decreasing function Ψ and some unknown admissible function Φ (see [Mat06]).

Bauer and Hohage have proposed another approach for applying the Lepskii principle for nonlinear inverse problems for regularized Newton methods (see [BH05]). The distance $d(a^\dagger, a_{\bar{i}})$ is there the radius of the smallest ball that contains $a^\dagger$, up to a constant (see [Mat06]).

The scheme which we use in our applications for determining the regularization parameter is going to be presented in detail in section 5.3.

5.2 Rates of convergence for Lepskii choice in deterministic setting

In this section we study the Lepskii choice of the regularization parameter and rates of convergence for the corresponding estimator for Tikhonov regularization in Hilbert scales in the same deterministic noise model as in section 2.4 and under Assumptions 4.4 on the operator F. Since we use the adaptive ideas presented in [PS05], we treat error terms $\|a_\alpha - a^\dagger\|$ (noise free error) and $\|a_\alpha^\delta - a_\alpha\|$ (data noise error) separately. We define the estimators a_α^δ as in (4.1) and a_α by

$$a_\alpha := \operatorname{argmin}_{a \in Q \cap (a_0 + \mathcal{X}_s)} \left(\|F(a) - u^\dagger\|_{\mathcal{Y}}^2 + \alpha \|a - a_0\|_s^2 \right) \tag{5.2}$$

where $s \geq 0$ and $a_0 \in H$ is an initial guess.

Theorem 5.4. *Let Assumptions 4.4 hold and let a_α be defined as above. Then we have the estimation*

$$\|a_\alpha - a^\dagger\|_{\mathcal{X}} \leq C\alpha^{\frac{q}{2(p+s)}}$$

with the constant C depending on $a^\dagger, p, q, s$.

Proof. As a_α is a solution of the minimization problem for the Tikhonov functional, the following inequality holds

$$\begin{aligned}\|F(a_\alpha)-u^\dagger\|_{\mathcal{Y}}^2+\alpha\|a_\alpha-a_0\|_s^2 &\le \|F(a^\dagger)-u^\dagger\|_{\mathcal{Y}}^2+\alpha\|a^\dagger-a_0\|_s^2\\ &=\alpha\|a^\dagger-a_0\|_s^2.\end{aligned}$$

It follows that

$$\begin{aligned}\|F(a_\alpha)-u^\dagger\|_{\mathcal{Y}}^2+\alpha\|a_\alpha-a^\dagger\|_s^2 &\le \alpha(\|a^\dagger-a_0\|_s^2+\|a_\alpha-a^\dagger\|_s^2-\|a_\alpha-a_0\|_s^2)\\ &=2\alpha\left\langle a^\dagger-a_0,a^\dagger-a_\alpha\right\rangle_s.\end{aligned}$$

From Assumption 3 (see (4.12)) it follows that

$$F(a_\alpha)=F(a^\dagger)+F'(a^\dagger)(a_\alpha-a^\dagger)+r_\alpha,\ \text{ with } \|r_\alpha\|_{\mathcal{Y}}\le\frac{\lambda^2}{4\Lambda}\|a_\alpha-a^\dagger\|_{-p}.$$

Replacing the difference $F(a_\alpha)-F(a^\dagger)$ in the previous inequality we obtain

$$\begin{aligned}\|F'(a^\dagger)(a_\alpha-a^\dagger)\|_{\mathcal{Y}}^2+\|r_\alpha\|_{\mathcal{Y}}^2+2\left\langle F'(a^\dagger)(a_\alpha-a^\dagger),r_\alpha\right\rangle+\alpha\|a_\alpha-a^\dagger\|_s^2&\\ \le 2\alpha\left\langle a^\dagger-a_0,a^\dagger-a_\alpha\right\rangle_s.&\end{aligned}\tag{5.3}$$

Using now Assumption 2 we get that

$$\lambda^2\|a_\alpha-a^\dagger\|_{-p}^2+\alpha\|a_\alpha-a^\dagger\|_s^2\le 2\Lambda\frac{\lambda^2}{4\Lambda}\|a_\alpha-a^\dagger\|_{-p}^2+2\alpha\left\langle a^\dagger-a_0,a^\dagger-a_\alpha\right\rangle_s.$$

Since we assumed that $a^\dagger-a_0\in\mathcal{X}_q$ we have that

$$\frac{\lambda^2}{2}\|a_\alpha-a^\dagger\|_{-p}^2+\alpha\|a_\alpha-a^\dagger\|_s^2\le 2c\alpha\|a_\alpha-a^\dagger\|_{2s-q}$$

where $c=\|L^q(a^\dagger-a_0)\|$. We apply the interpolation inequality (3.9) for $-p\le 2s-q\le s$ and obtain

$$\frac{\lambda^2}{2}\|a_\alpha-a^\dagger\|_{-p}^2+\alpha\|a_\alpha-a^\dagger\|_s^2\le 2c\alpha\|a_\alpha-a^\dagger\|_{-p}^{\frac{-s+q}{s+p}}\|a_\alpha-a^\dagger\|_s^{\frac{2s-q+p}{s+p}}.\tag{5.4}$$

Then

$$\|a_\alpha-a^\dagger\|_{-p}^2=\mathcal{O}\left(\alpha\|a_\alpha-a^\dagger\|_{-p}^{\frac{-s+q}{s+p}}\|a_\alpha-a^\dagger\|_s^{\frac{2s-q+p}{s+p}}\right)$$

and we choose in the Lemma 4.5 $r=2$, $t=\frac{-s+q}{s+p}$, $c=\|a_\alpha-a^\dagger\|_{-p}$, $d=\alpha\|a_\alpha-a^\dagger\|_s^{\frac{2s-q+p}{s+p}}$ and $e=0$ to get

$$\|a_\alpha-a^\dagger\|_{-p}^2=\mathcal{O}\left(\alpha^{\frac{2(s+p)}{3s+2p-q}}\|a_\alpha-a^\dagger\|_s^{\frac{2(2s-q+p)}{3s+2p-q}}\right).$$

From (5.4) it follows that

$$\begin{aligned}\|a_\alpha - a^\dagger\|_s^2 &= \mathcal{O}\left(\|a_\alpha - a^\dagger\|_s^{\frac{2s-q+p}{s+p}} \alpha^{\frac{-s+q}{3s+2p-q}} \|a_\alpha - a^\dagger\|_s^{\frac{(-s+q)(2s-q+p)}{(s+p)(3s+2p-q)}} \right) \\ &= \mathcal{O}\left(\alpha^{\frac{-s+q}{3s+2p-q}} \|a_\alpha - a^\dagger\|_s^{\frac{2(2s-q+p)}{3s+2p-q}} \right)\end{aligned}$$

and from Lemma 4.5 with $r = 2$, $t = \frac{2(2s-q+p)}{3s+2s-q}$, $c = \|a_\alpha - a^\dagger\|_s$, $d = \alpha^{\frac{-s+q}{3s+2p-q}}$, $e = 0$ we have that

$$\|a_\alpha - a^\dagger\|_s^2 = \mathcal{O}\left(\alpha^{\frac{-s+q}{s+p}} \right)$$

and

$$\|a_\alpha - a^\dagger\|_{-p}^2 = \mathcal{O}\left(\alpha^{\frac{p+q}{s+p}} \right). \tag{5.5}$$

Using the interpolation inequality (3.9) the desired rate of convergence is obtained

$$\begin{aligned}\|a_\alpha - a^\dagger\|_{\mathcal{X}} \leq \|a_\alpha - a^\dagger\|_{-p}^{\frac{s}{p+s}} \|a_\alpha - a^\dagger\|_s^{\frac{p}{s+p}} &\leq c\alpha^{\frac{1}{2}\frac{q}{p+s}} \\ &= \mathcal{O}\left(\alpha^{\frac{q}{2(p+s)}} \right).\end{aligned}$$

□

Theorem 5.5. *Under the assumptions of Theorem 5.4 we have that*

$$\|a_\alpha^\delta - a_\alpha\|_{\mathcal{X}} \leq c(\alpha^{\frac{-p}{2(p+s)}}\delta + \alpha^{\frac{q}{2(p+s)}})$$

with the constant c depending on C, p, q, s.

Proof. Let a_α^δ be a solution of the optimization problem (4.1). We notice that in the proof of Theorem 4.6 we did not use the fact that $\widehat{a}$ was actually the solution of the minimization problem (4.2), so we consider now the Lagrange -Euler equation for the optimization problem (4.1). From classical results for calculus of variations we know that the first variation of the Tikhonov functional J_α, defined in (4.1), is null for every direction $h \in X_s$ and, since J_α is Fréchet differentiable in a_α^δ it follows that ${J_\alpha}'(a_\alpha^\delta)h = 0$ for all $h \in \mathcal{X}_s$. This means

$$\left\langle F(a_\alpha^\delta) - Y^\delta, F'(a_\alpha^\delta)h \right\rangle + \alpha \left\langle a_\alpha^\delta - a_0, h \right\rangle_s = 0,\ h \in \mathcal{X}_s.$$

Due to the same arguments, since a_α is the solution of the minimization problem (5.2) and from the Lagrange-Euler equation it follows

$$\left\langle F(a_\alpha) - u^\dagger, F'(a_\alpha)h \right\rangle + \alpha \left\langle a_\alpha - a_0, h \right\rangle_s = 0,\ h \in \mathcal{X}_s.$$

As $a_\alpha^\delta - a_0, a_\alpha - a_0 \in \mathcal{X}_s$ we have that $a_\alpha^\delta - a_\alpha \in \mathcal{X}_s$ and we can choose the direction $h = a_\alpha^\delta - a_\alpha$ in both equalities. It follows that

$$\begin{aligned}
\left\langle F(a_\alpha^\delta) - Y^\delta, F'(a_\alpha^\delta)(a_\alpha^\delta - a_\alpha)\right\rangle + \alpha \left\langle a_\alpha^\delta - a_0, a_\alpha^\delta - a_\alpha\right\rangle_s = 0,\\
\left\langle F(a_\alpha) - u^\dagger, F'(a_\alpha)(a_\alpha^\delta - a_\alpha)\right\rangle + \alpha \left\langle a_\alpha - a_0, a_\alpha^\delta - a_\alpha\right\rangle_s = 0.
\end{aligned}$$

Taking the difference between these two relations we obtain

$$\begin{aligned}
&\left\langle F(a_\alpha^\delta) - Y^\delta, F'(a_\alpha^\delta)(a_\alpha^\delta - a_\alpha)\right\rangle - \left\langle F(a_\alpha) - u^\dagger, F'(a_\alpha)(a_\alpha^\delta - a_\alpha)\right\rangle\\
&+ \alpha \left\langle a_\alpha^\delta - a_\alpha, a_\alpha^\delta - a_\alpha\right\rangle_s = 0.
\end{aligned} \tag{5.6}$$

From Assumption 3 we can write the Taylor polynomial as

$$\begin{aligned}
F(a_\alpha) &= F(a^\dagger) + F'(a^\dagger)(a_\alpha - a^\dagger) + \int_0^1 \left\{F'(a^\dagger + t(a_\alpha - a^\dagger)) - F'(a^\dagger)\right\}(a_\alpha - a^\dagger)\, dt\\
F(a_\alpha^\delta) &= F(a^\dagger) + F'(a^\dagger)(a_\alpha^\delta - a^\dagger) + \int_0^1 \left\{F'(a^\dagger + t(a_\alpha^\delta - a^\dagger)) - F'(a^\dagger)\right\}(a_\alpha^\delta - a^\dagger)\, dt
\end{aligned}$$

and we get

$$\begin{aligned}
F(a_\alpha^\delta) - F(a_\alpha) = F'(a^\dagger)&(a_\alpha^\delta - a_\alpha)\\
&- \int_0^1 \left\{F'(a^\dagger + t(a_\alpha - a^\dagger)) - F'(a^\dagger)\right\}(a_\alpha - a^\dagger)\, dt\\
&+ \int_0^1 \left\{F'(a^\dagger + t(a_\alpha^\delta - a^\dagger)) - F'(a^\dagger)\right\}(a_\alpha^\delta - a_\alpha)\, dt\\
&+ \int_0^1 \left\{F'(a^\dagger + t(a_\alpha^\delta - a^\dagger)) - F'(a^\dagger)\right\}(a_\alpha - a^\dagger)\, dt.
\end{aligned}$$

We denote the three integrals as I_1, I_2 respectively I_3 and, from Assumption 3, we can bound their norms by

$$
\begin{aligned}
\|I_1\| &\le \int_0^1 \|F'(a^\dagger + t(a_\alpha - a^\dagger)) - F'(a^\dagger)\|_{\mathcal{Y}\leftarrow\mathcal{X}_{-p}} \|a_\alpha - a^\dagger\|_{-p}\, dt \\
&\le \int_0^1 C_L t \|a_\alpha - a^\dagger\| \|a_\alpha - a^\dagger\|_{-p}\, dt = \frac{C_L}{2}\|a_\alpha - a^\dagger\| \|a_\alpha - a^\dagger\|_{-p} \\
&\le \frac{\lambda^2}{4\Lambda}\|a_\alpha - a^\dagger\|_{-p} \\
\|I_2\| &\le \int_0^1 \|F'(a^\dagger + t(a_\alpha^\delta - a^\dagger)) - F'(a^\dagger)\|_{\mathcal{Y}\leftarrow X_{-p}} \|a_\alpha^\delta - a_\alpha\|_{-p}\, dt \\
&\le \int_0^1 C_L t \|a_\alpha^\delta - a^\dagger\| \|a_\alpha^\delta - a_\alpha\|_{-p}\, dt \le \frac{C_L}{2}\|a_\alpha^\delta - a^\dagger\| \|a_\alpha^\delta - a_\alpha\|_{-p} \\
&\le \frac{\lambda^2}{4\Lambda}\|a_\alpha^\delta - a_\alpha\|_{-p} \\
\|I_3\| &\le \int_0^1 \|F'(a^\dagger + t(a_\alpha^\delta - a^\dagger)) - F'(a^\dagger)\|_{Y\leftarrow X_{-p}} \|a_\alpha - a^\dagger\|_{-p}\, dt \\
&\le \int_0^1 C_L t \|a_\alpha^\delta - a^\dagger\| \|a_\alpha - a^\dagger\|_{-p}\, dt \le \frac{C_L}{2}\|a_\alpha^\delta - a^\dagger\| \|a_\alpha - a^\dagger\|_{-p} \\
&\le \frac{\lambda^2}{4\Lambda}\|a_\alpha - a^\dagger\|_{-p}.
\end{aligned}
$$

We write now the relation (5.6) as

$$
\begin{aligned}
&\left\langle F(a_\alpha^\delta) - F(a_\alpha) + F(a_\alpha) - u^\dagger + u^\dagger - Y^\delta, (F'(a_\alpha^\delta) - F'(a^\dagger))(a_\alpha^\delta - a_\alpha)\right\rangle \\
&- \left\langle F(a_\alpha) - u^\dagger, (F'(a_\alpha) - F'(a^\dagger))(a_\alpha^\delta - a_\alpha)\right\rangle \\
&+ \left\langle F(a_\alpha^\delta) - F(a_\alpha) - Y^\delta + u^\dagger, F'(a^\dagger)(a_\alpha^\delta - a_\alpha)\right\rangle + \alpha\|a_\alpha^\delta - a_\alpha\|_s^2 = 0.
\end{aligned}
$$

Using the Taylor formula we get

$$
\begin{aligned}
&\left\langle F'(a^\dagger)(a_\alpha^\delta - a_\alpha) - I_1 + I_2 + I_3 + F'(a^\dagger)(a_\alpha - a^\dagger) + I_1 + u^\dagger - Y^\delta,\right. \\
&\left.(F'(a_\alpha^\delta) - F'(a^\dagger))(a_\alpha^\delta - a_\alpha)\right\rangle + \alpha\|a_\alpha^\delta - a_\alpha\|_s^2 \\
&- \left\langle F'(a^\dagger)(a_\alpha - a^\dagger) + I_1, (F'(a_\alpha) - F'(a^\dagger))(a_\alpha^\delta - a_\alpha)\right\rangle \\
&+ \left\langle F'(a^\dagger)(a_\alpha^\delta - a_\alpha) - I_1 + I_2 + I_3 + u^\dagger - Y^\delta, F'(a^\dagger)(a_\alpha^\delta - a_\alpha)\right\rangle = 0.
\end{aligned}
$$

It follows

$$
\begin{aligned}
&\alpha\|a_\alpha^\delta - a_\alpha\|_s^2 + \|F'(a^\dagger)(a_\alpha^\delta - a_\alpha)\|_{\mathcal{Y}}^2 = \left\langle F'(a^\dagger)(a_\alpha - a^\dagger) + I_1, (F'(a_\alpha) - F'(a^\dagger))(a_\alpha^\delta - a_\alpha)\right\rangle \\
&- \left\langle -I_1 + I_2 + I_3 + u^\dagger - Y^\delta, F'(a^\dagger)(a_\alpha^\delta - a_\alpha)\right\rangle \\
&- \left\langle F'(a^\dagger)(a_\alpha^\delta - a_\alpha) + I_2 + I_3 + F'(a^\dagger)(a_\alpha - a^\dagger) + u^\dagger - Y^\delta, (F'(a_\alpha^\delta) - F'(a^\dagger))(a_\alpha^\delta - a_\alpha)\right\rangle.
\end{aligned}
$$

From Cauchy-Schwarz inequality, Assumptions (4.4) and (4.4) and the norm estimates for I_1, I_2 and I_3 we have

$$\begin{aligned}
&\lambda^2\|a_\alpha^\delta - a_\alpha\|_{-p}^2 + \alpha\|a_\alpha^\delta - a_\alpha\|_s^2 \\
&\leq \left(\Lambda\|a_\alpha - a^\dagger\|_{-p} + \frac{\lambda^2}{4\Lambda}\|a_\alpha - a^\dagger\|_{-p}\right)\frac{\lambda^2}{4\Lambda}\|a_\alpha^\delta - a_\alpha\|_{-p} \\
&+ \left(\frac{\lambda^2}{4\Lambda}\|a_\alpha - a^\dagger\|_{-p} + \frac{\lambda^2}{4\Lambda}\|a_\alpha^\delta - a_\alpha\|_{-p} + \frac{\lambda^2}{4\Lambda}\|a_\alpha - a^\dagger\|_{-p} + \delta\right)\Lambda\|a_\alpha^\delta - a_\alpha\|_{-p} \\
&+ \left(\delta + \Lambda\|a_\alpha^\delta - a_\alpha\|_{-p} + \frac{\lambda^2}{4\Lambda}\|a_\alpha^\delta - a_\alpha\|_{-p} + \Lambda\|a_\alpha - a^\dagger\|_{-p}\right. \\
&\left.+\frac{\lambda^2}{4\Lambda}\|a_\alpha - a^\dagger\|_{-p}\right)\frac{\lambda^2}{4\Lambda}\|a_\alpha^\delta - a_\alpha\|_{-p}.
\end{aligned}$$

We can rewrite this inequality as

$$\begin{aligned}
&\lambda^2\|a_\alpha^\delta - a_\alpha\|_{-p}^2 + \alpha\|a_\alpha^\delta - a_\alpha\|_s^2 \leq \left(\frac{\lambda^2}{2} + \frac{\lambda^4}{16\Lambda^2}\right)\|a_\alpha^\delta - a_\alpha\|_{-p}^2 + \\
&\left(\lambda^2 + \frac{\lambda^4}{8\Lambda^2}\right)\|a_\alpha - a^\dagger\|_{-p}\|a_\alpha^\delta - a_\alpha\|_{-p} + \left(\Lambda + \frac{\lambda^2}{4\Lambda}\right)\delta\|a_\alpha^\delta - a_\alpha\|_{-p}
\end{aligned} \tag{5.7}$$

As $\lambda \leq \Lambda$ we have that

$$\|a_\alpha^\delta - a_\alpha\|_{-p}^2 = \mathcal{O}\left(\|a_\alpha - a^\dagger\|_{-p}\|a_\alpha^\delta - a_\alpha\|_{-p} + \delta\|a_\alpha^\delta - a_\alpha\|_{-p}\right)$$

and this implies (using Lemma 4.5)

$$\|a_\alpha^\delta - a_\alpha\|_{-p}^2 = \mathcal{O}\left(\delta^2 + \|a_\alpha - a^\dagger\|_{-p}^2\right) = \mathcal{O}\left(\delta^2 + \alpha^{\frac{p+q}{s+p}}\right) \tag{5.8}$$

since we computed the rates of convergence for the approximation error $\|a_\alpha - a^\dagger\|_{-p}^2 = \mathcal{O}\left(\alpha^{\frac{p+q}{p+s}}\right)$ in the previous theorem (see Theorem 5.4).
Using (5.5) and (5.8) in (5.7) we notice that

$$\begin{aligned}
\|a_\alpha^\delta - a_\alpha\|_s^2 &= \mathcal{O}\left(\frac{1}{\alpha}(\|a_\alpha - a^\dagger\|_{-p}\|a_\alpha^\delta - a_\alpha\|_{-p} + \delta\|a_\alpha^\delta - a_\alpha\|_{-p})\right) \\
&= \mathcal{O}\left(\frac{1}{\alpha}\alpha^{\frac{1}{2}\frac{p+q}{p+s}}(\delta + \alpha^{\frac{1}{2}\frac{p+q}{p+s}}) + \frac{1}{\alpha}\delta(\delta + \alpha^{\frac{1}{2}\frac{p+q}{p+s}})\right) \\
&= \mathcal{O}\left(\delta\alpha^{\frac{q-2s-p}{2(s+p)}} + \alpha^{\frac{q-s}{p+s}} + \frac{\delta^2}{\alpha}\right).
\end{aligned}$$

We apply now the interpolation inequality (see (3.9)) to obtain

$$
\begin{aligned}
\|a_\alpha^\delta - a_\alpha\|_{\mathcal{X}}^2 &\le \|a_\alpha^\delta - a_\alpha\|_{-p}^{\frac{2s}{p+s}} \|a_\alpha^\delta - a_\alpha\|_s^{\frac{2p}{p+s}} \\
&= \mathcal{O}\left((\delta^{\frac{2s}{s+p}} + \alpha^{\frac{p+q}{p+s}\frac{s}{s+p}})(\delta^{\frac{p}{s+p}}\alpha^{\frac{q-2s-p}{2(s+p)}\frac{p}{s+p}} + \alpha^{\frac{q-s}{p+s}\frac{p}{s+p}} + \delta^{\frac{2p}{s+p}}\alpha^{\frac{-p}{s+p}}) \right) \\
&= \mathcal{O}\Bigg(\delta^{1+\frac{s}{s+p}}\alpha^{\frac{p(q-2s-p)}{2(s+p)^2}} + \delta^{\frac{2s}{s+p}}\alpha^{\frac{p(q-s)}{(s+p)^2}} + \delta^2\alpha^{-\frac{p}{s+p}} + \delta^{\frac{p}{s+p}}\alpha^{\frac{2sq+pq-p^2}{2(s+p)^2}} \\
&\quad + \alpha^{\frac{q}{p+s}} + \delta^{\frac{2p}{s+p}}\alpha^{\frac{qs-p^2}{(s+p)^2}} \Bigg).
\end{aligned}
$$

We now apply four times the Young inequality

$$ab \le \frac{a^k}{k} + \frac{b^l}{l},$$

which holds for all $a, b > 0$, $1 < k, l < \infty$ and $\frac{1}{k} + \frac{1}{l} = 1$ with $a^k = \delta^2\alpha^{\frac{-p}{s+p}}$. For the firm term we take $b = \alpha^{\frac{pq}{2(s+p)^2}}$, $k = \frac{2(s+p)}{2s+p}$ and $l = \frac{2(s+p)}{p}$, for the second $b = \alpha^{\frac{pq}{(s+p)^2}}$, $k = \frac{s+p}{s}$ and $l = \frac{s+p}{p}$, for the fourth $b = \alpha^{\frac{2qs+pq}{2(s+p)^2}}$, $k = \frac{2(s+p)}{p}$ and $l = \frac{2(s+p)}{2s+p}$ and for the sixth term $b = \alpha^{\frac{qs}{(s+p)^2}}$, $k = \frac{s+p}{p}$ and $l = \frac{s+p}{s}$. This yields

$$\|a_\alpha^\delta - a_\alpha\|_{\mathcal{X}}^2 = \mathcal{O}\left(\delta^2\alpha^{-\frac{p}{s+p}} + \alpha^{\frac{q}{p+s}} \right).$$

□

Theorem 5.6. *Under the assumptions of Theorems 5.4 and 5.5 it holds*

$$\|a_\alpha^\delta - a^\dagger\|_{\mathcal{X}} \le C^*(\delta\alpha^{\frac{-p}{2(s+p)}} + \alpha^{\frac{q}{2(p+s)}}).$$

The choice of the regularization parameter $\alpha^\dagger = \delta^{\frac{2(p+s)}{p+q}}$ *gives the order optimal rate of convergence*

$$\|a_{\alpha^\dagger}^\delta - a^\dagger\|_{\mathcal{X}} \le 2C^*\alpha^{\frac{q}{p+q}}.$$

Proof. The first inequality follows immediately from Theorems 5.4 and 5.5. For $\alpha = \alpha^\dagger = \delta^{\frac{2(p+s)}{p+q}}$ we get

$$\|a_\alpha^\delta - a^\dagger\|_{\mathcal{X}}^2 \le 2C^*(\delta^{\frac{2(p+s)}{p+q}})^{\frac{q}{p+q}} = 2C^*\delta^{\frac{2q}{p+q}}.$$

□

We discuss now the choice of the regularization parameter α based on the Lepskii principle and the previous bound for the total error $\|a_\alpha^\delta - a^\dagger\|$. We follow here the approach from [MP03] and [LPR07], where the notion of admissible functions was used (see also [Mat06]). This scheme chooses the regularization parameter α from a finite set of possible parameters

$$M = \left\{\alpha_1 = \delta^2, \alpha_j = \alpha_1 (q^2)^{j-1}, j = 2, \dots, m, \text{ with } m = \min\{k : \alpha_k \geq 1\}\right\}$$

with $q > 1$. We denote $a^\delta_{\alpha_j} = a_j$. Then the function

$$\Psi(j) = C^* \delta \alpha_j^{\frac{-p}{2(s+p)}}, j = 1, \dots, m$$

is decreasing and, as

$$\Psi(j+1) = C^* \delta \alpha_{j+1}^{\frac{-p}{2(s+p)}} = q^{\frac{-p}{2(s+p)}} \Psi(j)$$

it fulfills also the condition

$$q\Psi(j+1) = q^{\frac{2s+p}{2(s+p)}} \Psi(j) \geq \Psi(j).$$

The strategy consists in computing successively $\alpha_1, \alpha_2, \dots$ until we determine $\alpha_+ = \alpha_{i_+}$ such that

$$i_+ = \max\left\{ i : \|a_i - a_j\| \leq 4C^* \delta \alpha_j^{\frac{-p}{2(s+p)}}, j = 1, 2, \dots, i \right\}.$$

Theorem 5.7. *Under the hypothesis of Theorem (5.4) and (5.5) and for the choice of the regularization parameter $\alpha = \alpha_+$, the order-optimal error bound*

$$\|a_+ - a^\dagger\| \leq 6C^* \alpha^{\frac{q}{p+q}}.$$

holds true, where $a_+ = a_{\alpha_+}$.

Proof. The theorem is a direct consequence of Corollary 5.2.

Remark 5.8. *In [PS05] a simplified version of Lepskii criterion was presented, which had the origins in the quasi-optimality choice of the regularization parameter created by Tikhonov and Glasko. In this case we choose the index*

$$i_\diamond = \max\left\{ i : \|a_j - a_{j-1}\| \leq 4C^* \delta \alpha_j^{\frac{-p}{2(s+p)}}, j = 1, 2, \dots, i \right\}$$

and the estimator $a_\diamond = a_{\alpha_{i_\diamond}}$ corresponding to the regularization parameter $\alpha_\diamond = \alpha_{i_\diamond}$. From the definitions of i_+ and $i_\diamond$ it follows that $\alpha_* \leq \alpha_{i_+} \leq \alpha_{i_\diamond}$ and the *order optimal rate of convergence holds also for $a_\diamond$ since*

$$\begin{aligned}
\|a_\diamond - a^\dagger\| &\le \|a_* - a^\dagger\| + \sum_{j=i_*+1}^{i_\diamond} \|a_{\alpha_j-1} - a_j\| \\
&\le \|a_* - a^\dagger\| + 4C^*\delta \sum_{j=i_*+1}^{i_\diamond} \frac{1}{\alpha_{j-1}^{\frac{p}{2(s+p)}}} \\
&= \|a_* - a^\dagger\| + 4C^*\delta \sum_{j=0}^{i_\diamond - i_* - 1} \frac{1}{\alpha_*^{\frac{p}{2(s+p)}} q^j} \\
&\le 2C^*\delta\alpha_*^{\frac{-p}{2(s+p)}} + \frac{4C^*\delta}{\alpha_*^{\frac{p}{2(s+p)}}} \frac{1 - \frac{1}{q^{i_\diamond - i_+}}}{1 - \frac{1}{q}} \\
&\le 2C^*\delta\alpha_*^{\frac{-p}{2(s+p)}} (1 + 2\frac{1}{1 - \frac{1}{q}}) \\
&\le 6C^*\delta\alpha_*^{\frac{-p}{2(s+p)}} = 6C^*\delta^{\frac{q}{(p+q)}}.
\end{aligned}$$

5.3 Rates of convergence for Lepskii choice in stochastic setting

We return now to the stochastic case and to the notations from section 4.2, with the difference that we emphasize the dependance of the estimator $\widehat{a}$ on the regularization parameter α by writing $\widehat{a} = \widehat{a}_\alpha$. We choose the set of regularization parameters as

$$M := \left\{\alpha_j = \beta^2 (q^2)^{j-1}, j = 2, \ldots, \min\{k : \alpha_k \ge 1\}\right\}$$

with $q > 1$ and the estimator $\widehat{a}_+ = \widehat{a}_{\alpha_{i_+}}$ with

$$i_+ = \max\left\{i : \|\widehat{a}_i - \widehat{a}_j\| \le 4C^* \sqrt{\frac{2q}{p+q} \ln \frac{1}{\beta}} \beta \alpha_j^{\frac{-p}{2(s+p)}}, j = 1, 2, \ldots, i\right\}$$

where $\widehat{a}_i = \widehat{a}_{\alpha_i}$. The rates of convergence for this estimator can be computed using similar techniques as in [BP05, Bau04].

Theorem 5.9. *If, besides the Assumptions 4.4, the tail of the probability distribution for the estimator $\widehat{u}$ fulfills the condition*

$$\mathbf{P}\left\{\omega : \|\widehat{u} - \mathbf{E}\widehat{u}\|^2 \ge (\tau - 1)\mathbf{E}\left(\|\widehat{u} - \mathbf{E}\widehat{u}\|^2\right)\right\} \le k \exp(-\tau) \qquad (5.9)$$

for any $\tau > 1$ and for a constant $k > 0$, then, for all $\beta \leq \exp(-1)$, we have the following error bound for $\widehat{a}_+$

$$\mathbf{E}(\|\widehat{a}_+ - a^\dagger\|^2) \leq K^* \beta^{\frac{2q}{p+q}} \ln \frac{1}{\beta}$$

where K^* is a constant depending on k, p, q, λ, Λ, C_L and C^*.

Proof. We denote

$$\Omega_\tau = \left\{ \|\widehat{u} - u^\dagger\|^2 \geq \tau \mathbf{E}\left(\|\widehat{u} - u^\dagger\|^2\right)\right\}.$$

Due to Cauchy-Schwarz inequality we have the following implications

$$\begin{aligned}
&\|\widehat{u} - u^\dagger\|^2 \geq \tau \mathbf{E}\|\widehat{u} - u^\dagger\|^2 \\
\Leftrightarrow &\|\widehat{u} - \mathbf{E}\widehat{u} + \mathbf{E}\widehat{u} - u^\dagger\|^2 \geq \tau \mathbf{E}\|\widehat{u} - \mathbf{E}\widehat{u} + \mathbf{E}\widehat{u} - u^\dagger\|^2 \\
\Leftrightarrow &\|\widehat{u} - \mathbf{E}\widehat{u}\|^2 + 2\left\langle \widehat{u} - \mathbf{E}\widehat{u}, \mathbf{E}\widehat{u} - u^\dagger\right\rangle + \|\mathbf{E}\widehat{u} - u^\dagger\|^2 \geq \tau(\mathbf{E}\|\widehat{u} - \mathbf{E}\widehat{u}\|^2 \\
&+ 2\mathbf{E}\left\langle \widehat{u} - \mathbf{E}\widehat{u}, \mathbf{E}\widehat{u} - u^\dagger\right\rangle + \|\mathbf{E}\widehat{u} - u^\dagger\|^2) \\
\Rightarrow &\|\widehat{u} - \mathbf{E}\widehat{u}\|^2 + 2\left\langle \widehat{u} - \mathbf{E}\widehat{u}, \mathbf{E}\widehat{u} - u^\dagger\right\rangle + \|\mathbf{E}\widehat{u} - u^\dagger\|^2 \geq \tau \mathbf{E}\|\widehat{u} - \mathbf{E}\widehat{u}\|^2 + \tau\|\mathbf{E}\widehat{u} - u^\dagger\|^2 \\
\Rightarrow &\|\widehat{u} - \mathbf{E}\widehat{u}\|^2 + 2\|\widehat{u} - \mathbf{E}\widehat{u}\|\|\mathbf{E}\widehat{u} - u^\dagger\| + \|\mathbf{E}\widehat{u} - u^\dagger\|^2 \geq \tau \mathbf{E}\|\widehat{u} - \mathbf{E}\widehat{u}\|^2 + \tau\|\mathbf{E}\widehat{u} - u^\dagger\|^2 \\
\Rightarrow &\|\widehat{u} - \mathbf{E}\widehat{u}\|^2 + \frac{1}{\tau - 1}\|\widehat{u} - \mathbf{E}\widehat{u}\|^2 + (\tau - 1)\|\mathbf{E}\widehat{u} - u^\dagger\|^2 + \|\mathbf{E}\widehat{u} - u^\dagger\|^2 \\
&\geq \tau \mathbf{E}\|\widehat{u} - \mathbf{E}\widehat{u}\|^2 + \tau\|\mathbf{E}\widehat{u} - u^\dagger\|^2 \\
\Rightarrow &\|\widehat{u} - \mathbf{E}\widehat{u}\|^2 \geq (\tau - 1)\mathbf{E}\|\widehat{u} - \mathbf{E}\widehat{u}\|^2.
\end{aligned}$$

Therefore, we get

$$\mathbf{P}(\Omega_\tau) \leq k \exp(-\tau). \tag{5.10}$$

With the help of conditional expectation we can write

$$\mathbf{E}(\|\widehat{a}_+ - a^\dagger\|^2) = \mathbf{P}(\Omega_\tau)\mathbf{E}(\|\widehat{a}_+ - a^\dagger\|^2|\Omega_\tau) + \mathbf{P}(\mathbf{C}\Omega_\tau)\mathbf{E}(\|\widehat{a}_+ - a^\dagger\|^2|\mathbf{C}\Omega_\tau).$$

We apply the deterministic convergence result for Lepskii choice of the regularization parameter (see Theorem 5.7) on the set $\mathbf{C}\Omega_\tau$ for $\tau = \frac{2q}{p+q}\ln\frac{1}{\beta}$ and use the exponential inequality (5.10) to bound $\mathbf{P}(\Omega_\tau)$. This yields

$$\begin{aligned}
\mathbf{E}(\|\widehat{a}_+ - a^\dagger\|^2) &\leq k\exp(-\tau)\frac{\lambda^2}{2\Lambda C_L} + (1 - \mathbf{P}(\Omega_\tau))6C^* q(\tau\beta^2)^{\frac{q}{p+q}} \\
&\leq K\left(\exp(-\frac{2q}{p+q}\ln\frac{1}{\beta}) + \left(\beta^2\frac{2q}{p+q}\ln\frac{1}{\beta}\right)^{\frac{q}{p+q}}\right) \\
&\leq K\left(\beta^{\frac{2q}{p+q}} + \left(\frac{2q}{p+q}\right)^{\frac{q}{p+q}}\beta^{\frac{2q}{p+q}}\left(\ln\frac{1}{\beta}\right)^{\frac{q}{p+q}}\right) \\
&\leq K^*\beta^{\frac{2q}{p+q}}\ln\frac{1}{\beta}
\end{aligned}$$

since $\ln(\frac{1}{\beta}) \geq 1$ for $\beta \leq \exp(-1)$. $\square$

Remark 5.10. *The behavior of the tail of the probability distribution for different nonparametric estimators* $\widehat{u}$ *has been studied and can be computed for local polynomial estimators or wavelets (see e.g. [Mas96, Mas97]). It is then possible to choose in the first step of the algorithm an estimator with known asymptotical rates of ESE and with known tail-behavior.*

Remark 5.11. *Like in the deterministic setting, we can choose a simplified version for the choice of the regularization parameter. We use in our numerical simulations*

$$i_\diamond = \max\left\{ i : \|\widehat{a}_j - \widehat{a}_{j-1}\| \le 4C^* \sqrt{\frac{2q}{p+q} \ln \frac{1}{\beta}} \beta \alpha_j^{\frac{-p}{2(s+p)}}, j = 1, 2, \ldots, i \right\}$$

and we select the estimator $\widehat{a}_\diamond = \widehat{a}_{\alpha_{i_\diamond}}$*. In the same way as in the Theorem 5.9 we can prove that the rate of convergence is equal to*

$$\mathbf{E}(\|\widehat{a}_\diamond - a^\dagger\|^2) \le K \beta^{\frac{2q}{p+q}} \ln \frac{1}{\beta}.$$

Chapter 6

Applications

In this chapter we discuss the applicability of our results to some model examples arising from practical problems. A lot of applications in physics, biology or chemistry can be investigated as parameter identification problems, therefore the first two examples are modeled as inverse problems with the help of the parameter-to-solution mapping F. Numerous applications are also shaped as integral equations, hence in the last example F is a Hammerstein integral operator. The aim of this chapter is to construct the appropriate Hilbert scales based on the knowledge of the adjoint of the Fréchet derivative of the operator F and to check the Assumptions 4.4, especially the relation (4.4). The reconstruction of a reaction coefficient is typical example for a nonlinear inverse problem and we present here in detail the properties of the operator that we study, we motivate the choice of the Hilbert scale and we prove the relation (4.4). In the second example, we construct the Hilbert scale as the Friedrichs extension of the embedding between the two spaces $\mathcal{X}_0$ and $\mathcal{X}_1$ and we prove Assumptions 4.4. In the last example we present exhaustively the ideas from [Neu00]. Since the conditions of Theorem 4.6 are fulfilled, the estimator (4.2) is order-optimal for our applications.

6.1 Reconstruction of a reaction coefficient

Diffusion processes are described by differential equations of the form

$$\frac{\partial u}{\partial t}(t,x) = \mathbf{div}\alpha(x)\mathbf{grad}u(t,x) + f(x).$$

The unknown solution u may describe (as a function of time t and position x) a temperature, the concentration of a gas, a population density of a biological species or the piezometric head in groundwater filtration. If the coefficient functions α and f do not depend on t, then the solution $u(t,x)$ typically converges rapidly with $t \to \infty$ to a steady state solution $u(x)$ satisfying

$$-\mathbf{div}\alpha(x)\mathbf{grad}u(x) = f(x).$$

In this section we consider the case that the source term f is an affine linear function of the solution u, i.e. $f = \tilde{f} - au$. E.g. if chemical reactions occur in a gas, then f is a polynomial in u, in the simplest case of degree 1. In biology a linear dependence of the rate of change on a population density u is referred to as Malthus model. The proportionality constant a may depend on other parameters, in particular explicitly or implicitly on the space variable x. Replacing $\tilde{f}$ again by f and assuming $\alpha \equiv 1$ we arrive at the differential equation

$$-\Delta u(x) + a(x)u(x) = f(x), \quad x \in \Omega \tag{6.1}$$

where $\Omega \subseteq \mathbf{R}^d$, $d \in \{1, 2, 3\}$ is open, bounded and smooth. The forward problem to find u given a and f is completed by the boundary condition

$$u(x) = g(x), \quad x \in \partial\Omega.$$

The inverse problem we are going to study in the following consists in estimating a from measurements of u with known f and g. For simplicity we will assume f and g to be infinitely smooth. For a given bound $\gamma > 0$ we introduce the set

$$D(F) = \{a \in L^2(\Omega) : 0 \leq a \leq \gamma\}. \tag{6.2}$$

It follows from classical results on elliptic partial differential equations (see e.g. [Wlo87]) that for $a \in D(F)$ and $g \in H^{\frac{3}{2}}(\partial\Omega)$ there exists a unique solution $u_a \in H^2(\Omega)$ of the direct problem (6.1). We formulate the inverse problem of identifying the parameter $a \in L^2(\Omega)$ knowing $u_a = u_a(x)$ as an operator equation with the help of parameter-to-solution operator

$$F : D(F) \to L^2(\Omega), \quad F(a) := u_a. \tag{6.3}$$

In this section the Hilbert scale $(\mathcal{X}_s)_{s\in\mathbf{R}}$ will be generated by the square root $T(1)^{\frac{1}{2}}$ of the positive, self-adjoint operator $T(1)$ defined in Example 3.19.

Remark 6.1. *We saw in Example 3.23 that the first elements of this Hilbert scale with integer index are given by*

$$\mathcal{X}_1 = H_0^1(\Omega), \quad \mathcal{X}_2 = H_2(\Omega) \cap H_0^1(\Omega), \quad \mathcal{X}_3 = \{v \in H_3(\Omega) : v, \Delta v \in H_0^1(\Omega)\}.$$

This sheds some light on role of the initial guess a_0 in Theorem 4.6. For condition (4.7) to be fulfilled for a large index q, it is not sufficient that $a^\dagger$ and a_0 be smooth (e.g. C^∞), but additionally the boundary values of $a^\dagger$ and its derivatives must be known a-priori. This a-priori knowledge (if available) must be incorporated in the initial guess a_0. We have observed in numerical experiments that such a-priori knowledge of the behavior of $a^\dagger$ at the boundary is also necessary for fast convergence.

In the following analysis the operator $T(a)$ defined in Example 3.19 will play a dominant role. In the following lemma we are going to establish some properties of these operators, following ideas from [CK86].

Lemma 6.2. *There exist two strictly positive constants k_1 and k_2 such that*

$$k_1\|v\|_{\mathcal{X}_2} \leq \|T(a)v\|_{L^2(\Omega)} \leq k_2\|v\|_{\mathcal{X}_2} \tag{6.4a}$$

$$k_1\|v\|_{L^2(\Omega)} \leq \|T(a)v\|_{\mathcal{X}_{-2}} \leq k_2\|v\|_{L^2(\Omega)} \tag{6.4b}$$

for all $v \in H^2(\Omega) \cap H_0^1(\Omega)$ and all $a \in D(F)$.
Furthermore, there exists a positive constant C such that

$$\| \left(T(a)^{-1} - T(\overline{a})^{-1}\right) \varphi\|_{\mathcal{X}_2} \leq C\|a - \overline{a}\|_{L^2(\Omega)}\|\varphi\|_{L^2(\Omega)}. \tag{6.5}$$

for any $a, \overline{a} \in D(F)$, $\varphi \in L^2(\Omega)$.

Proof. The existence of a constant k_2 independent of a in (6.4a) is easily seen from the definition of the operator $T(a)$ as

$$\begin{aligned}
\|T(a)v\| &\leq \| \triangle v\|_{L^2(\Omega)} + \|av\|_{L^2(\Omega)} \\
&\leq \| \triangle v\|_{L^2(\Omega)} + \gamma\|v\|_{L^2(\Omega)} \\
&\leq \max(1, \gamma)\|v\|_{H^2(\Omega)}.
\end{aligned}$$

Now we prove the first inequality in (6.4a) where the constant k_1 is also independent of $a \in D(F)$. The L^2-norm of $T(a)v$ can be estimated from below by

$$\begin{aligned}
\|T(a)v\|^2_{L^2(\Omega)} &= \int_\Omega \left(- \triangle v + av\right)^2 \, dx \\
&= \int_\Omega \left((\triangle v)^2 - 2av \triangle v + a^2v^2\right) \, dx \\
&\geq \| \triangle v\|^2_{L^2(\Omega)} - 2\int_\Omega |av \triangle v| \, dx + \int_\Omega a^2v^2 \, dx.
\end{aligned} \tag{6.6}$$

From the inequality $2|av \triangle v| \leq 4a^2v^2 + \dfrac{(\triangle v)^2}{4}$ we have that

$$\begin{aligned}
\|T(a)v\|^2_{L^2(\Omega)} &\geq \| \triangle v\|^2_{L^2(\Omega)} - \int_\Omega \frac{(\triangle v)^2}{4} \, dx - \int_\Omega 4a^2v^2 \, dx + \int_\Omega a^2v^2 \, dx \\
&\geq \frac{3}{4}\| \triangle v\|^2_{L^2(\Omega)} - 3\int_\Omega a^2v^2 \, dx \\
&\geq \frac{3}{4}\| \triangle v\|^2_{L^2(\Omega)} - 3\gamma^2\|v\|^2_{L^2(\Omega)}
\end{aligned} \tag{6.7}$$

On the other hand

$$\langle T(a)v, v\rangle = \int_\Omega (- \triangle v + av) \, v \, dx = \int_\Omega | \bigtriangledown v|^2 + av^2 \, dx \geq \int_\Omega | \bigtriangledown v|^2 \, dx \geq \frac{1}{k}\|v\|^2_{H^1}.$$

where k is the Poincaré constant and is independent of $v \in H_0^1(\Omega)$. Applying Cauchy-Schwarz inequality we obtain that

$$\frac{1}{k}\|v\|_{L^2(\Omega)}^2 \leq \frac{1}{k}\|v\|_{H^1}^2 \leq \|T(a)v\|_{L^2(\Omega)}\|v\|_{L^2(\Omega)}$$

and hence

$$\frac{1}{k}\|v\|_{L^2(\Omega)} \leq \|T(a)v\|_{L^2(\Omega)}. \tag{6.8}$$

Multiplying the squared inequality (6.8) by $3\gamma^2k^2$ and adding this to (6.7) yields

$$\left(1+3\gamma^2k^2\right)\|T(a)v\|_{L^2(\Omega)}^2 \geq \|\triangle v\|_{L^2(\Omega)}^2 \geq K^2\|v\|_{H^2(\Omega)}^2$$

using the global regularity result $\|\triangle u\|_{L^2(\Omega)} \geq K\|u\|_{H^2(\Omega)}$ with constant K independent of $u \in H^2(\Omega) \cap H_0^1(\Omega)$. This completes the proof of the first inequality in (6.4a).
(6.4b) follows from (6.4a) and Lemma 3.5 below since $T(a)$ is self- adjoint with respect to the L^2- norm and boundedly invertible from $\mathcal{X}_2$ to $\mathcal{X}_0$.
In order to prove (6.5) we consider the difference

$$v = \left(T(a)^{-1} - T(\overline{a})^{-1}\right)\varphi = v_a - v_{\overline{a}}$$

where $v_a = T(a)^{-1}\varphi$ and $v_{\overline{a}} = T(\overline{a})^{-1}\varphi$. As

$$T(a)v = \varphi - T(a)v_{\overline{a}} = (T(\overline{a}) - T(a))v_{\overline{a}} = (\overline{a} - a)\,v_{\overline{a}},$$

it follows that

$$\begin{aligned}\|v\|_{\mathcal{X}_2} &= \|T(a)^{-1}(\overline{a}-a)\,v_{\overline{a}}\|_{\mathcal{X}_2} \leq k_1^{-1}\|(\overline{a}-a)\,v_{\overline{a}}\|_{L^2(\Omega)} \\ &\leq k_1^{-1}\|a-\overline{a}\|_{L^2(\Omega)}\|v_{\overline{a}}\|_\infty \leq ck_1^{-1}\|a-\overline{a}\|_{L^2(\Omega)}\|v_{\overline{a}}\|_{\mathcal{X}_2} \\ &\leq ck_1^{-2}\|a-\overline{a}\|_{L^2(\Omega)}\|\varphi\|_{L^2(\Omega)}.\end{aligned}$$

□

We will assume that the exact solution $u^\dagger = u_{a^\dagger}$ of the equation (6.1) fulfills the condition

$$c_u = \inf_{x\in\Omega} u^\dagger(x) > 0 \tag{6.9}$$

which is satisfied if $g > 0$ and $f \geq 0$ by the maximum principle.

Theorem 6.3. *If (6.9) holds true, then F satisfies Assumption 4.4 for $s \geq 2$.*

Proof. The Fréchet differentiability of F has been established in [CK86, CK89]. Injectivity follows easily from (6.9) as the relation $u_a = u^\dagger$ implies $(a - a^\dagger)u^\dagger = 0$ for any $a \in D(F)$. Since $D(F) \cap (a_0 + \mathcal{X}_s)$ is closed and convex for $s \geq 2$, it is weakly sequentially closed. Hence, for a weakly convergent sequence $(a_n)_{n\in\mathbf{N}}$ in $D(F)\cap(a_0+\mathcal{X}_s)$ the limit point a belongs to $D(F)\cap(a_0+\mathcal{X}_s)$. Since $d\le 3$, it follows from the compactness of the embedding $\mathcal{X}^s\hookrightarrow\mathcal{X}^{7/4}$ and the continuity of the embedding $\mathcal{X}^{7/4}\hookrightarrow L^\infty(\Omega)$ that there exists a weakly convergent subsequence (a_{n_k}) in $L^\infty(\Omega)$. Since F is continuous (even Fréchet differentiable) on $L^\infty(\Omega)$, it follows that $\|F(a_{n_k})-F(a)\|_{\mathcal{Y}}\to 0$ as $k\to\infty$. This shows that F is weakly sequentially closed. $\square$

Differentiating (6.1) with respect to a shows that the Fréchet derivative $F'(a)h=v_h$ is the unique solution v_h of the equation

$$T(a)v_h=-hu_a \tag{6.10}$$

where u_a is the solution of (6.1). Hence, the adjoint of the Fréchet derivative is given by

$$F'(a)^*\varphi=-u_aT(a)^{-1}\varphi \tag{6.11}$$

where $\varphi\in L^2(\Omega)$.

Theorem 6.4. *If assumption (6.9) holds true and $(\mathcal{X}_s)_{s\in\mathbf{R}}$ is the Hilbert scale generated by $\sqrt{T(1)}$, then F' satisfies Assumption 4.4 with $p=2$. Moreover, Assumption 4.4 is satisfied if γ in (6.2) is sufficiently small.*

Proof. To prove Assumption 4.4 we use the chain of inequalities (6.4b) and the relation (6.10). It follows that

$$\|F'(a)h\|_{L^2(\Omega)}=\|T(a)^{-1}\left(-hu_a\right)\|_{L^2(\Omega)}\sim\|hu_a\|_{\mathcal{X}_{-2}} \tag{6.12}$$

with constants independent of a. From the Banach algebra property for the Sobolev space $H^m(\Omega)$(see [AF03] for details) it holds that

$$\|vw\|_{H^m(\Omega)}\le K\|v\|_{H^m(\Omega)}\|w\|_{H^m(\Omega)} \tag{6.13}$$

where $u,v\in H^m(\Omega)$, Ω is a domain in $\mathbf{R}^d$ satisfying the cone condition, $2m>d$ and the constant K depends on m,d and the cone determining the cone condition for Ω. Choosing $m=2$ and $d=1,2,3$ in (6.13) we have

$$\|vw\|_{H^2(\Omega)}\le K\|v\|_{H^2(\Omega)}\|w\|_{H^2(\Omega)} \tag{6.14}$$

and from relation (3.4) the multiplication operator $M_{u_a}:h\to hu_a$ has bounded norm

$$\|M_{u_a}\|_{\mathcal{X}_{-2}\leftarrow\mathcal{X}_{-2}}=\|M_{u_a}\|_{\mathcal{X}_2\leftarrow\mathcal{X}_2}\le K\|u_a\|_{H^2(\Omega)}. \tag{6.15}$$

Due to (6.9), $\|\frac{1}{u_a}\|_{H^2(\Omega)}$ is finite, and hence

$$\|M_{u_a}^{-1}\|_{\mathcal{X}_{-2}\leftarrow\mathcal{X}_{-2}}=\|M_{u_a}^{-1}\|_{\mathcal{X}_2\leftarrow\mathcal{X}_2}\le K\|\frac{1}{u_a}\|_{H^2(\Omega)}<\infty.$$

This implies $\|hu_a\|_{\mathcal{X}_{-2}} \sim \|h\|_{\mathcal{X}_{-2}}$. Together with (6.12) this finishes the proof of Assumption 4.4. In Lemma 3.5 we consider the Gelfand triples $X_2 \subset L^2(\Omega) \subset X_{-2}$ and $L^2(\Omega) \subset L^2(\Omega) \subset L^2(\Omega)$ with the function $F'(a) : X_{-2} \to L^2(\Omega)$ and the adjoint $F'(a)^* : L^2(\Omega) \to L^2(\Omega)$. Due to (3.4), it suffices to show Lipschitz continuity of the mapping $a \to F'(a)^*$ from $\mathcal{X}_0$ to $L\left(L^2\left(\Omega\right), \mathcal{X}_2\right)$ to prove Assumption 4.4. From eq. (6.11) we can write

$$[F'(a)]^* = M_{u_a} \circ T(a)^{-1}.$$

It is going to be proved now that

$$\|(M_{u_a} \circ T(a)^{-1} - M_{u_{\overline{a}}} \circ T(\overline{a})^{-1})\varphi\|_{\mathcal{X}_2} \leq c\|\varphi\|_{L^2(\Omega)}\|a - \overline{a}\|_{L^2(\Omega)}$$

where c is a constant which can vary from now on. We split the difference in two terms which can be estimated

$$\begin{aligned}&\|(M_{u_a} \circ T(a)^{-1} - M_{u_{\overline{a}}} \circ T(\overline{a})^{-1})\varphi\|_{\mathcal{X}_2} \\ \leq &\|M_{u_a}[T(a)^{-1} - T(\overline{a})^{-1}]\varphi\|_{\mathcal{X}_2} + \|(M_{u_a} - M_{u_{\overline{a}}})T(\overline{a})^{-1}\varphi\|_{\mathcal{X}_2}.\end{aligned} \tag{6.16}$$

The first term on the right hand side of the inequality (6.16) can be bounded using (6.5) and (6.15). If $Z : H^{\frac{3}{2}}\left(\partial\Omega\right) \to H^2\left(\Omega\right)$ is a right inverse of the trace operator, we have $F(a) = u_a = \tilde{u}_a + Zg$ with $\tilde{u}_a = T(a)^{-1}\left(f - Zg\right)$ and $F(\overline{a}) = u_{\overline{a}} = \tilde{u}_{\overline{a}} + Zg$ and $\tilde{u}_{\overline{a}} = T(\overline{a})^{-1}\left(f - Zg\right)$. It follows from Lemma 6.2 that

$$\begin{aligned}\|u_a - u_{\overline{a}}\|_{\mathcal{X}_2} &= \|\left(T(a)^{-1} - T(\overline{a})^{-1}\right)\left(f - Zg\right)\|_{\mathcal{X}_2} \\ &\leq C\|a - \overline{a}\|_{L^2(\Omega)}\|f - Zg\|_{L^2(\Omega)}.\end{aligned}$$

Together with the Banach algebra property (6.14) and (6.4a) we obtain

$$\begin{aligned}\|(M_{u_a} - M_{u_{\overline{a}}})T(\overline{a})^{-1}\varphi\|_{\mathcal{X}_2} &= \|(u_a - u_{\overline{a}})T(\overline{a})^{-1}\varphi\|_{\mathcal{X}_2} \leq \frac{K}{k_1}\|u_a - u_{\overline{a}}\|_{\mathcal{X}_2}\|\varphi\|_{L^2(\Omega)} \\ &\leq \left(\frac{CK}{k_1}\|f - Zg\|_{L^2(\Omega)}\right)\|a - \overline{a}\|_{L^2(\Omega)}\|\varphi\|_{L^2(\Omega)}.\end{aligned}$$

This proves that our operator satisfies Assumption 4.4. □

For the direct regression problem in the first step we have to determine the precise regularity of $u^\dagger$:

Proposition 6.5. *If $a^\dagger \in H^q(\Omega)$ with $q > d/2$, then $u^\dagger \in H^{q+2}(\Omega)$.*

Proof. The regularity result can be derived as follows from standard elliptic regularity estimates where smoothness of $a^\dagger$ is measured in terms of L^∞ based Sobolev spaces of integer order: By Sobolev's embedding theorem we have $a^\dagger \in W^{q-d/2-\epsilon,\infty}(\Omega)$ for any $\epsilon > 0$, and in particular $a^\dagger \in W^{k,\infty}(\Omega)$ with $k := \sup\{\tilde{k} \in$

$\mathbf{N}_0 : \tilde{k} < q - d/2\}$ (see [RR04]). By standard elliptic regularity estimates we get $u^\dagger \in H^{k+2}(\Omega)$. To improve this regularity, we rewrite the differential equation as

$$-\Delta u = \tilde{f} \qquad \text{with} \qquad \tilde{f} := f - au.$$

Since f is assumed to be smooth and $q, k+2 > d/2$, we have $\tilde{f} \in H^{\min(k+2,q)}(\Omega)$ due to (6.13). First assume that $k+2 \geq q$. Then $u^\dagger \in H^{q+2}(\Omega)$ by regularity results for Poisson's equation. If $k+2 < q$, we have to repeat the last argument to further improve the regularity of $u^\dagger$. □

Definition 6.6. *Assume the noise model (2.9), let the assumptions of Theorem 6.4 hold true, let $s \geq 2$, $q \in [s, 2s+2]$, and assume that $a^\dagger - a_0 \in \mathcal{X}_q$ and $a^\dagger \in H^q(\Omega)$. Then $u^\dagger$ can be estimated such that (1.5) holds true with $\beta \sim \sigma^{\frac{q}{q+2+d/2}}$. Moreover, for the choice $\alpha \sim \sigma^{\frac{2q(2+s)}{(q+2+d/2)(2+q)}}$ we get*

$$\sqrt{\mathbf{E}\|\widehat{a} - a^\dagger\|^2_{L^2(\Omega)}} = \mathcal{O}\left(\sigma^{\frac{q}{q+2+d/2}}\right), \qquad \sigma \to 0.$$

Proof. The first statement follows from Proposition 6.5 and general results from nonparametric regression (see [Tsy04]). The second statement is a consequence of Theorems 4.6, 6.3 and 6.4. □

6.2 Reconstruction of a diffusion coefficient

The second application is the 1−dimensional, steady-state case of the groundwater flow equation. A general form of the equation describing the transient flow of a compressible fluid in a non-homogeneous, anisotropic aquifer is

$$\frac{\partial}{\partial x_i}\left(a_{ij}\frac{\partial u}{\partial x_i}\right) = S_s\frac{\partial u}{\partial t} + f,\ i, j = 1, \ldots, 3$$

where S_s is the specific storage, t is the time, f is the volumetric flux per unit volume (positive for outflow and negative for inflow) due to sink and water sources, a_{ij} is the specific diffusivity of the sediment layer and u is the hidraulic head. Aquifer properties can vary spatially and fluid properties can vary in space and time. We consider here the 1−dimensional, steady-state case of the groundwater flow equation

$$\begin{cases} -(au')' = f \text{ on } (0,1), \\ u(0) = g_0, \quad u(1) = g_1. \end{cases} \tag{6.17}$$

Here the parameter a belongs to the set of admissible functions $D(F) = \{q \in H^2((0,1)) : \underline{\gamma} \leq q, \|q\|_{H^2} \leq \gamma\}$ with strictly positive constants $\underline{\gamma}$ and γ and f is a smooth function. Under these assumptions there exists a unique weak solution u_a to (6.17) for a given parameter a, and u_a belongs to the Sobolev space of functions $H^2 = H^2(0,1)$ (see Definition 3.7). In the following we will always omit the

domain $(0,1)$ in function spaces. Our inverse problem of identifying the parameter a in the boundary value problem (6.17) is formulated as an operator equation (1.1) with the parameter-to-solution operator $F : D(F) \to L^2$, $F(a) = u_a$.
It turns out that Assumption 4.4 is neither satisfied for the Hilbert scale generated by the Dirichlet Laplacian nor the Hilbert scale generated by the shifted Neumann Laplacian. Therefore, we introduce a different Hilbert scale starting from the space

$$L^2_\diamond := \left\{ v \in L^2 : \int_0^1 v\,dx = 0 \right\}$$

and the operator

$$\begin{aligned} \overline{B} : D(\overline{B}) = \left\{ u \in H^2 : u'(0) = u'(1) = 0, \int_0^1 u\,dx = 0 \right\} \to L^2_\diamond, \\ \overline{B}\phi := -\phi'' + \phi. \end{aligned} \tag{6.18}$$

$\overline{B}$ is well defined as

$$\int_0^1 \overline{B}\phi\,dx = \int_0^1 (-\phi'' + \phi)\,dx = -\phi'(1) + \phi'(0) + \int_0^1 \phi\,dx = 0.$$

$\overline{B}$ is also densely defined, as H^2 is dense in L^2. It is also easy to see that $\overline{B}$ is symmetric, as for any $\varphi, \phi \in D(\overline{B})$ we have

$$\begin{aligned} \langle \overline{B}\phi, \varphi \rangle &= \int_0^1 (-\phi'' + \phi)\varphi\,dx = (-\phi'\varphi)\mid_0^1 + \int_0^1 \phi'\varphi'\,dx + \int_0^1 \phi\varphi\,dx \\ &= (\phi\varphi')\mid_0^1 - \int_0^1 \phi\varphi''\,dx + \int_0^1 \phi\varphi\,dx = \langle \phi, \overline{B}\varphi \rangle. \end{aligned}$$

It follows that the operator $(D(\overline{B}^*), \overline{B}^*)$ is an extension of $(D(\overline{B}), \overline{B})$, so $D(\overline{B}) \subseteq D(\overline{B}^*)$. $\overline{B}$ is self-adjoint if $D(\overline{B}) = D(\overline{B}^*)$. As the operator $(D(\overline{B}), \overline{B})$ is bijective (see [Tay96a, Prop. 5.7.5]), it follows from [Tay96a, Prop. A 8.3] that $\overline{B}$ is also self-adjoint. Moreover, $\overline{B}$ is strictly positive as

$$\langle \overline{B}\phi, \phi \rangle = \int_0^1 (\phi'^2 + \phi^2)\,dx \geq \|\phi\|_{L^2}.$$

First we consider the Hilbert scale $\left(\widehat{X}_s\right)_{s \in \mathbf{R}}$ generated by the operator $\overline{B}^{\frac{1}{2}}$. However, to prove Assumption 4.4 we need $\mathcal{X}$ to be a subspace of H^1, so we choose the shifted scale

$$\mathcal{X}_s = \widehat{\mathcal{X}}_{s+1} \tag{6.19}$$

which is also a Hilbert scale (see e.g. [EHN96, Prop. 8.19]). The first integer elements of this scale are given by

$$\begin{aligned} &\mathcal{X}_{-1} = L^2_\diamond, \qquad \mathcal{X}_0 = H^1_\diamond := H^1 \cap L^2_\diamond, \qquad \mathcal{X}_1 = D(\overline{B}), \\ &\mathcal{X}_2 = H^3 \cap D(\overline{B}), \qquad \mathcal{X}_3 = \{\phi \in H^4 \cap D(\overline{B}) : \phi'''(0) = \phi'''(1) = 0\}. \end{aligned} \tag{6.20}$$

We introduce the orthogonal projection $P_\diamond : L^2 \to L^2_\diamond$, $v \mapsto v - \int_0^1 v\,dx$ and the embedding operator $J_\diamond : H^1_\diamond \hookrightarrow L^2_\diamond$. $J_\diamond$ is injective and, due to the density of H^1 in L^2, has also dense range. This also implies that its adjoint $J^*_\diamond : L^2_\diamond \to H^1_\diamond$ is injective and has dense range. By [Neu88, Prop. 2.1] it follows that

$$J^*_\diamond f = \overline{B}^{-1} f \tag{6.21}$$

for $f \in L^2_\diamond$. We notice also that $\overline{B} = (J_\diamond J^*_\diamond)^{-1}$, hence $\overline{B}$ is the Friedrich extension of $J_\diamond$ in $L^2_\diamond$ (see Theorem 3.11).
We assume that the exact solution $u^\dagger$ of the direct problem (6.17) fulfills the condition

$$\inf_{x\in(0,1)} |u^{\dagger'}(x)\,| > 0. \tag{6.22}$$

Theorem 6.7. *If (6.22) holds true, then F satisfies Assumption 4.4 for $s \geq 2$.*

Proof. Under assumption (6.22) the injectivity of the operator F follows immediately from [Kun88, Theorem 2.1]. Due to similar arguments as in section 6.1 the operator F is weakly sequentially closed between $D(F) \cap (a_0 + \mathcal{X}_s)$, $s \geq 2$ and L^2 for $s \geq 2$ (see [BHM04]). The Fréchet differentiability of F has been established in [CK89]. ☐

In order to prove the Assumptions 4.4 and 4.4 we will use the operator $T(a) : H^2 \cap H^1_0 \to L^2$ defined in Example 3.8 which is self-adjoint as a densely defined operator on L^2. The Fréchet derivative $F'(a)h = \eta$ for a given perturbation $h \in H^1$ of a is the weak solution of the equation

$$\begin{cases} -(a\eta')' = (hu'_a)', \\ \eta(0) = \eta(1) = 0 \end{cases} \tag{6.23}$$

(see [CK89]). Hence, F' can be written in operator form as

$$F'(a)h = S(a) D_x M_{u'_a} J_\diamond h \tag{6.24}$$

where $M_{u'_a} : L^2_\diamond \to L^2$, $h \mapsto u'_a h$ is a multiplication operator, $D_x : L^2 \to H^{-1}$ is the differentiation operator, and $S(a) : H^{-1} \to L^2$ maps $f \in H^{-1}$ to the solution of the boundary value problem (6.23) with $(hu'_a)'$ replaced by f. (Note that actually the range of $S(a)$ is contained in H^1_0!) To compute $F'(a)^* : L^2 \to H^1_\diamond$ we have to find the adjoint of each factor in (6.24). Since $T(a)$ is self-adjoint in L^2, the adjoint of $S(a)$ with respect to the Gelfand triple $H^{-1} \subset L^2 \subset H^1_0$ is given by $S(a)^* : L^2 \to H_0^1$, $S(a)^*\varphi = T(a)^{-1}\varphi$. Moreover, $M_{u_a'}^* v = P_\diamond(u_a' \cdot v)$. From eq. (6.21) we get

$$F'(a)^*\varphi = -\overline{B}^{-1} P_\diamond \left\{u_a'[T(a)^{-1}\varphi]'\right\}, \qquad \varphi \in L^2. \tag{6.25}$$

In order to prove the Assumptions 4.4 and 4.4 we need the following properties of $T(a)$.

Lemma 6.8. *For all $a \in H^2 \cap D(F)$ there exists two positive constants k_1 and k_2 such that*

$$k_1\|v\|_{H^2} \leq \|T(a)v\|_{L^2} \leq k_2\|v\|_{H^2}. \tag{6.26}$$

for $v \in H^2$, where k_1 and k_2 can be chosen independent of a. Furthermore, there exists a positive constant C such that

$$\|\left(T(a)^{-1} - T(\overline{a})^{-1}\right)\varphi\|_{H^2} \leq C\|a-\overline{a}\|_{H^1}\|\varphi\|_{L^2}. \tag{6.27}$$

for any $a, \overline{a} \in D(F)$, $\varphi \in L^2(\Omega)$.

Proof. The second inequality is easily seen from

$$\|-(av')'\|_{L^2} \leq \|av'\|_{H^1} \leq K\|a\|_{H^1}\|v'\|_{H^1} \leq K\gamma\|v\|_{H^2}$$

where we used that

$$\|uv\|_{H^1} \leq K\|u\|_{H^1}\|v\|_{H^1} \tag{6.28}$$

for $u, v \in H^1$ and $K > 0$ independent of u and v (see (6.13)). The constant $k_2 = K\gamma$ is independent of a.
For the first inequality we use the elliptic a-priori estimate for the solution of equation $T(a)v = f$

$$\|v\|_{H^2} \leq C\left(\|v\|_{H^1} + \|f\|_{L^2}\right) a_{n_k}$$

with C depending on $\underline{\gamma}$ and $\|a\|_{W^{1,\infty}}$ (see e.g. [GT83, Theorem 8.13]). Since H^2 is continuously embedded in $W^{1,\infty}$, C depends only on $\underline{\gamma}$ and γ, but not on a. Multiplying in (6.17) by a test function $w \in H_0^1$ and integrating by parts, yields

$$l(v, w; a) = \int_0^1 fw\,dx \tag{6.29}$$

with the bilinear form $l(.,.;a) : H_0^1 \times H_0^1 \to \mathbf{R}$ given by

$$l(v, w; a) = \int_0^1 a(x)\,v' \cdot w'\,dx.$$

It follows from Poincaré's inequality that l satisfies the inequality

$$k\|v\|_{H^1}^2 \le l(v,v;a) \tag{6.30}$$

for all $a \in D(F)$, $v \in H_0^1$, where k is a constant that depends on $\underline{\gamma}$ and the Poincaré constant. Moreover, $l(v,v;a) = \int_0^1 fv\,dx \le \|f\|_{L^2}\|v\|_{L^2} \le \|f\|_{L^2}\|v\|_{H^1}$. Hence, the solution v to (6.17) fulfills

$$\|v\|_{H^1} \le k^{-1}\|f\|_{L^2}$$

and first statement is proved. (6.27) can be proved considering the difference

$$v = \left(T(a)^{-1} - T(\overline{a})^{-1}\right)\varphi = v_a - v_{\overline{a}}$$

where $v_a = T(a)^{-1}\varphi$ and $v_{\overline{a}} = T(\overline{a})^{-1}\varphi$. As

$$T(a)v = \varphi - T(a)v_{\overline{a}} = (T(\overline{a}) - T(a))v_{\overline{a}} = ((\overline{a}-a)\,v'_{\overline{a}})'$$

it follows that

$$\begin{aligned}\|v\|_{H^2} &= \|T(a)^{-1}\left((\overline{a}-a)\,v'_{\overline{a}}\right)'\|_{H^2} \le k_1^{-1}\|\left((\overline{a}-a)\,v'_{\overline{a}}\right)'\|_{L^2} \le Kk_1^{-1}\|a-\overline{a}\|_{H^1}\|v'_{\overline{a}}\|_{H^1}\\ &\le Kk_1^{-1}\|a-\overline{a}\|_{H^1}\|v_{\overline{a}}\|_{H^2} \le Kk_1^{-2}\|a-\overline{a}\|_{H^1}\|\varphi\|_{L^2}.\end{aligned}$$

□

As a preparation for the next theorem we rewrite (6.25) as

$$F'(a)^*\varphi = -\overline{B}^{-1}AT(a)^{-1}\varphi, \qquad \varphi \in L^2 \tag{6.31}$$

with the operator

$$A : H^2 \cap H_0^1 \to H_\diamond^1, \qquad v \mapsto P_\diamond({u^\dagger}' \cdot v').$$

Lemma 6.9. *The operator A is an isomorphism between $H^2 \cap H_0^1$ and $H_\diamond^1$.*

Proof. From the definition of A as the composition of three linear and bounded operators, we have that A is also linear and bounded. We prove now that A is injective. Let $v \in H^2 \cap H_0^1$ be such that $Av = 0$. It follows that $P_\diamond({u^\dagger}'v') = 0$, which means ${u^\dagger}'v' = c$ with $c := \int_0^1 {u^\dagger}'(x)v'(x)\,dx$. Then $v' = \frac{c}{{u^\dagger}'}$. But from the Mean Value Theorem, as $v(0) = v(1) = 0$ there exists $\xi \in (0,1)$ such that $v'(\xi) = 0$. Hence, $c = 0$, $v = 0$ and A is injective.
Next we prove that A is a Fredholm operator of index zero. The projection $P_\diamond : H^1 \to H_\diamond^1$ is a Fredholm operator of index 1 since it is surjective and its kernel consists only of the constant functions. As the operator $M_{{u^\dagger}'}$ is bijective due to the assumption (6.22), it is a Fredholm operator, and its index is zero. To

prove that $D_x : H^2 \cap H_0^1 \to H^1$ is a Fredholm operator we consider the bounded linear operator

$$E : H^1 \to H_0^1 \cap H^2, \qquad (Ev)(x) := \int_0^x (P_\diamond v)(t)\, dt.$$

Since $P_\diamond D_x u = u' - \int_0^1 u'\, dx = u' - u(1) + u(0) = u'$ for $u \in H^2 \cap H_0^1$, we have

$$ED_x u = u, \qquad \text{and} \qquad D_x E v = P_\diamond v$$

for $v \in H^1$. Since E is surjective and its kernel consists of the constant functions, E is Fredholm with $\operatorname{ind}(E) = 1$. Moreover, E is a Fredholm inverse of D_x, and hence D_x is Fredholm with $\operatorname{ind}(D_x) = -\operatorname{ind}(E_x) = -1$.
As a composition of Fredholm operators A is also a Fredholm operator, and its index is

$$\operatorname{ind}(A) = \operatorname{ind}(P_\diamond) + \operatorname{ind}(M_{u^{\dagger\prime}}) + \operatorname{ind}(D_x) = 1 + 0 - 1 = 0.$$

Together with the injectivity of A shown in first part of the proof this yields the assertion. $\square$

Theorem 6.10. *If (6.22) holds true and the Hilbert scale is defined as in (6.19) then Assumptions 4.4 holds true for* $p = 2$. *Moreover, Assumption 4.4 is satisfied if the diameter of* $D(F) \cap (a_0 + \mathcal{X}_s)$ *with respect to the* $\mathcal{X}$*-norm is sufficiently small.*

Proof. To prove Assumption 4.4 we actually show that $\|F'(a^\dagger)^*\varphi\|_{\mathcal{X}_2} \sim \|\varphi\|_{L^2}$ using Lemma (6.9) and (6.26). As $F'(a^\dagger)^*$ is a composition of three isomorphisms, the norm-equivalence follows immediately. The proof of Assumption 4.4 follows the steps of the proof of Theorem 6.4. We apply again Lemma 3.5, and, using (6.25) we get

$$\begin{aligned}
&\|F'(a)^*\varphi - F'(\overline{a}^*)\varphi\|_{\mathcal{X}_2} = \left\| P_\diamond u_a' \left(T(a)^{-1}\varphi\right)' - P_\diamond u_{\overline{a}}' \left(T(\overline{a})^{-1}\varphi\right)' \right\|_{\mathcal{X}_0} \\
&\le \|P_\diamond\|_{\mathcal{X}_0 \leftarrow H^1} \left\{ \left\| u_a' \left(T(a)^{-1}\varphi - T(\overline{a})^{-1}\varphi\right)' \right\|_{\mathcal{X}_0} + \left\| (u_a' - u_{\overline{a}}') \left(T(a)^{-1}\varphi\right)' \right\|_{\mathcal{X}_0} \right\}.
\end{aligned} \tag{6.32}$$

Since $u_a = \tilde{u}_a + g$ and $u_{\overline{a}} = \tilde{u}_{\overline{a}} + g$ with $g(x) := g_0 + x(g_1 - g_0)$, $\tilde{u}_a := T(a)^{-1}(f-g)$, and $\tilde{u}_{\overline{a}} := T(\overline{a})^{-1}(f-g)$, it follows from Lemma 6.8 that

$$\begin{aligned}
\|u_a' - u_{\overline{a}}'\|_{H^1} &\le \|u_a - u_{\overline{a}}\|_{H^2} = \|\left(T(a)^{-1} - T(\overline{a})^{-1}\right)(f-g)\|_{H^2} \\
&\le C\|a - \overline{a}\|_{H^1}\|f - g\|_{L^2}.
\end{aligned}$$

Therefore, the second term on the right hand side of (6.32) is bounded by a multiple of $\|a - \overline{a}\|_{H^1}\|\varphi\|_{L^2}$. Using the Banach algebra property (6.28) and (6.27) the first term on the right hand side of (6.32) can be bounded by $c\|a - \overline{a}\|_{H^1}\|\varphi\|_{L^2}$ as well. $\square$

Proposition 6.11. *If $a^\dagger \in H^{q+1}$ with $q > \frac{1}{2}$, then $u^\dagger \in H^{q+2}$.*

Proof. It follows from the differential equation (6.17) that

$$u^{\dagger\prime} = \frac{\overline{f}}{a^\dagger}$$

where $\overline{f}$ is a primitive of f. As $a^\dagger \in D(F)$ is bounded from below, it follows that $1/a^\dagger \in H^{q+1}$. Hence, $u^{\dagger\prime} = \overline{f}/a^\dagger \in H^{q+1}$ since f is assumed to be smooth (see (6.13)). It follows that $u^\dagger \in H^{q+2}$. □

Let us summarize our results:

Definition 6.12. *In the case of the noise model (2.9), if the assumptions of Theorem (6.10) hold true and if $s \geq 2$, $q \in [s, 2s+2]$, $a^\dagger - a_0 \in \mathcal{X}_q$, and $a^\dagger \in H^{q+1}$, then $u^\dagger$ can be estimated such that (1.5) holds true with $\beta \sim \sigma^{\frac{q+2}{q+2+1/2}}$. Moreover, for the choice $\alpha \sim \sigma^{\frac{2(2+s)}{(q+2+1/2)}}$ we get*

$$\begin{aligned} \sqrt{\mathbf{E}\|\widehat{a} - a^\dagger\|_{H^1}^2} &= \mathcal{O}\left(\sigma^{\frac{q}{q+2+1/2}}\right), \\ \sqrt{\mathbf{E}\|\widehat{a} - a^\dagger\|_{L^2}^2} &= \mathcal{O}\left(\sigma^{\frac{q+1}{q+2+1/2}}\right). \end{aligned}$$

Proof. The first statement follows from Proposition 6.11 and well-known results from nonparametric regression (see [Tsy04]). The second statement is a consequence of Remark 4.7 with $r = 0$ and $r = -1$ and Theorems 6.7 and 6.10. □

From the characterization of the elements of the Hilbert scale $(\mathcal{X}_s)_{s\in\mathbf{R}}$ (see 6.20), it follows that for fast rates of convergence $a^\dagger$ must be smooth, and additionally the mean value of $a^\dagger$ and its odd derivatives at the boundary must be known and incorporated in the initial guess a_0.

6.3 Hammerstein operator

The next application that we consider is a non-linear integral equation. A systematical development of a theory for equations of the type

$$a(t) = \int_\Omega k(t,s)\Phi(s, a(s))\, ds$$

was realized by Hammerstein in 1930. A possible motivation to study this problem was that of the forced oscillation of finite amplitude of a pendulum

$$a''(t) + \omega \sin a(t) = f(t), \quad t \in [0,1]$$

where $a(t)$ represents the elongation at time t, ω is the angular frequency and f is the forcing term. For an odd function f, this differential equation can be converted to a Hammerstein integral equation

$$a(s) = -\int_0^1 T(s,t)[f(t) - \omega^2 \sin a(t)]\, dt$$

where $T(s,t)$ is the Green function for the Laplacian with homogeneous Dirichlet boundary conditions (see [Ans64]). Applications can be found not only in elasticity theory but also in fluids theory and plasma physics (see [Mor02]).
We consider here the Hammerstein operator

$$\begin{aligned} F : H^1 &\to L^2 \\ a &\mapsto \int_0^\bullet \Phi(a(t))\, dt \end{aligned} \tag{6.33}$$

where Φ is a function in the space of Hölder continuous functions $C^{2,1}(\mathbf{R})$ with bounded second derivative

$$\|\Phi''(t)\|_{C^{0,1}} \leq K \tag{6.34}$$

for all $t \in \mathbf{R}$ and H^1 again denotes the Sobolev space of index 1 of functions on the interval $[0,1]$. Our inverse problem is to determine a from the knowledge of $F(a)$. As we mentioned in section 4.2 similar Assumptions as in 4.4 were used in [EN05] to study the Landweber iterative method in Hilbert scales. This example was inspired by [Neu00].

Lemma 6.13. *F is a continuous, compact, weakly closed and Fréchet differentiable operator with the Fréchet derivative*

$$(F'(a)h)(t) = \int_0^t \Phi'(a(s))h(s)\, ds \tag{6.35}$$

The adjoint of the Fréchet derivative is given by

$$F'(a)^* g = B^{-1}\left(\Phi'(a(\cdot))\int_\bullet^1 g(s)\, ds\right). \tag{6.36}$$

Here $B : \{v \in H^2 : v'(0) = v'(1) = 0\} \to L^2$ is defined by $Bv := -v'' + v$.

Proof. F is the composition of the Nemitzkii operator $\overline{\Phi} : H^1 \to L^2, \overline{\Phi}(a) = \Phi \circ a$ and the linear integral operator $A : L^2 \to L^2, (Af)(x) = \int_0^x f(t)\, dt$.
We study first the properties of the operator $\overline{\Phi}$. We want to prove now that $\overline{\Phi}$ is weakly sequentially closed. Let $a_n \rightharpoonup a$ in H^1, $\overline{\Phi}(a_n) \rightharpoonup u$ in L^2. From Rellich's embedding theorem it follows that $a_n \to a$ in L^2. Furthermore, there exists a subsequence a_{k_n} that converges pointwise to a. Since Φ is continuous, we have

that $\Phi(a_{k_n}) \to \Phi(a)$ pointwise as $n \to \infty$. As a_n is a weakly convergent sequence in H^1, it is also bounded in H^1 and, from Sobolev's embedding theorem it follows that there exist positive constants C_1 and C_2 such that

$$\|a_{k_n}\|_\infty \leq C_1 \|a_{k_n}\|_{H^1} \leq C_2.$$

Moreover, since Φ is continuous, it holds

$$\|\overline{\Phi}(a_{k_n})\|_\infty \leq \tilde{C}$$

for all $n \geq 1$ and for a constant $\tilde{C}$. We can apply now Lebesgue's dominated convergence theorem to the subsequence $\overline{\Phi}(a_{k_n})$, to show that it converges to $\overline{\Phi}(a)$ also in L^2. This proves that $\overline{\Phi}$ is weakly sequentially closed.
To prove Fréchet differentiability we use Taylor formula

$$\Phi(y) - \Phi(x) = \Phi'(x)(y-x) + \frac{\Phi''(\xi)}{2}(y-x)^2 \tag{6.37}$$

with ξ a number between x and y, $x, y \in \mathbf{R}$. We consider $a, h \in H^1$, $t \in [0,1]$ and write

$$\Phi\left((a+h)(t)\right) - \Phi(a(t)) - \Phi'(a(t))h(t) = \frac{\Phi''(\xi)}{2} h^2(t)$$

with ξ between $a(t)$ and $a(t) + h(t)$. We use the bound on the function Φ'' to write down

$$|\Phi\left((a+h)(t)\right) - \Phi(a(t)) - \Phi'(a(t))| \leq K|h(t)|^2.$$

Due to the continuous embedding of H^1 in the space of continuous functions which implies $\|h\|_\infty \leq C\|h\|_{H^1}$ we can conclude

$$\|\overline{\Phi}(a+h) - \overline{\Phi}(a) - (\Phi' \circ a)h\|_{L^2}^2 \leq M \int_0^1 |h(t)|^4 \, dt \leq MC^4 \|h\|_{H^1}^4 = \mathcal{O}\left(\|h\|_{H^1}^4\right).$$

It follows that the Fréchet derivative of $\overline{\Phi}$ at a is $\overline{\Phi}'(a) : H^1 \to L^2, \overline{\Phi}'(a)h = (\Phi' \circ a)h$.
Results regarding the linear integral operator A can be found for example in [PS90] or [Kre89]. As an integral operator with L^2 kernel, A is bounded, compact, and it is not only weakly closed but also strongly continuous (see [Zei90, Proposition 21.29]).
F is the composition between $\overline{\Phi}$ and A, so it is continuous, weakly closed and Fréchet differentiable. From the chain rule we get the Fréchet derivative

$$F'(a) : H^1 \to L^2,\ (F'(a)h)(t) = \left(A \circ \overline{\Phi}'(a)\right)(h)(t) = \int_0^t \Phi'(a(s))h(s)\, ds.$$

In Example 3.2 we saw that the adjoint of A is

$$A^* : L^2 \to L^2,\ A^*(v)(s) = \int_s^1 v(t)\,dt$$

and it is clear that the adjoint of $\overline{\Phi}'(a)$ is

$$(\overline{\Phi}'(a))^* : L^2 \to H^1,\ \overline{\Phi}'(a)^* h = j^*(\Phi' \circ a)h.$$

where $j : H^1 \hookrightarrow L^2$ is the embedding of H^1 in L^2. Since $j^* = B^{-1}$, it follows that

$$F'(a)^*(h) = B^{-1}(\Phi' \circ a)(\cdot) \int_{\cdot}^1 h(s)\,ds).$$

□

We assume now that

$$\Phi'(s) > 0,\ \text{for all } s \in \mathbf{R}. \tag{6.38}$$

Injectivity of F follows immediately. Due to Remark 3.29 we determine the set $R(F'(a^\dagger)^*)$ in order to choose a Hilbert scale which fulfills Assumptions 4.4 and 4.4. $F'(a^\dagger)^*$ is the composition of three operators: A^*, the multiplication operator $M_{\Phi' \circ a^\dagger} : L^2 \to L^2$, $M_{\Phi' \circ a^\dagger}(h) = (\Phi' \circ a^\dagger)h$ and B^{-1}. The operator $A^* : L^2 \to L^2$, $A^*(g)(s) = \int_s^1 g(t)\,dt$ has the range

$$R(A^*) = \left\{u \in H^1 : u(1) = 0\right\}$$

and

$$M(\Phi' \circ a^\dagger)(R(A^*)) = \left\{u \in H^1 : u(1) = 0\right\}$$

as $\Phi' \circ a^\dagger$ is in H^1. Note that due to (6.38) there exists $\gamma > 0$ such that

$$\frac{1}{\gamma} \le \Phi'(a^\dagger(s)) \le \gamma$$

for all $s \in [0,1]$ since $\|a^\dagger\|_\infty < \infty$. Since the restriction

$$\tilde{B} := B|_{D(B)\cap H^3} : \left\{v \in H^3 : v'(0) = v'(1) = 0\right\} \to H^1$$

is an isomorphism by elliptic regularity results and since $(Bv)(1) = 0$ is equivalent to $v''(1) = v(1)$ we finally get

$$R(F'(a^\dagger)^*) = R(B^{-1} \circ M_{\Phi' \circ a^\dagger} \circ A^*) = \left\{v \in H^3 : v'(0) = v'(1) = 0, v(1) = v''(1)\right\}.$$

As the operators $A^*, M(\Phi' \circ a^\dagger)$ and B^{-1} are injective, we have that $F'(a^\dagger)^*$ is bijective between L^2 and $R(F'(a^\dagger)^*)$ and $\|F'(a^\dagger)^* w\|_{H^3} \sim \|w\|_{L^2}$ for all $w \in L^2$.

We would like to have a Hilbert scale $\{\mathcal{X}_s\}_{s\in\mathbf{R}}$ with the following properties: We need

$$\mathcal{X}_0 = H^1 \tag{6.39a}$$

(or higher regularity of $\mathcal{X}_0$) to be able to show (4.4), and we need $R(F'(a^\dagger)^*)$ to be a member of the Hilbert scale, e.g.

$$\mathcal{X}_2 = \{w \in H^3 : w'(0) = w'(1) = 0, w(1) = w''(1)\} \tag{6.39b}$$

$$\langle w, v\rangle_{\mathcal{X}_2} = \left\langle \widetilde{B}w, \widetilde{B}v \right\rangle_{H^1} = \int_0^1 w^{(3)}v^{(3)} + 3w''v'' + 3w'v' + wv\,dx. \tag{6.39c}$$

Unfortunately, the restriction $\widetilde{B} : R(F'(a^\dagger)^*) \to H^1$ is not self-adjoint and we need to consider another operator that generates the Hilbert scale.

Proposition 6.14. *The operator*

$$\begin{aligned} L : D(L) = \{w \in H^5 : w'(0) = w'(1) = w^{(3)}(0) = 0, w(1) = w''(1)\} \to H^1 \\ Lw := w - 2w'' + w^{(4)}. \end{aligned}$$

is self-adjoint in H^1, and

$$D(L^{\frac{1}{2}}) = R(F'(a^\dagger)^*). \tag{6.40}$$

Proof. We are going to prove that L is the Friedrichs extension of the embedding of $R(F'(a^\dagger)^*) \hookrightarrow H^1$ (see Theorem 3.12). First we remark that for $w \in D(L)$ and $v \in R(F'(a^\dagger)^*)$ we have that

$$\begin{aligned} \langle Lw, v\rangle_{H^1} =& \int_0^1 (w^{(4)} - 2w'' + w)v + (w^{(5)} - 2w^{(3)} + w')v'\,dx \qquad (6.41) \\ =& w^{(3)}(1)v(1) - w^{(3)}(0)v(0) - \int_0^1 w^{(3)}v'\,dx - 2w'(1)v(1) + 2w'(0)v(0) \\ &+ 2\int_0^1 w'v'\,dx + \int_0^1 wv\,dx + w^{(4)}(1)v'(1) - w^{(4)}(0)v'(0) - \int_0^1 w^{(4)}v''\,dx \\ &- 2w''(1)v'(1) + 2w''(0)v'(0) + 2\int_0^1 w''v''\,dx + \int_0^1 w'v'\,dx \\ =& w^{(3)}(1)v(1) - w''(1)v'(1) + w''(0)v'(0) + \int_0^1 w''v''\,dx + 3\int_0^1 w'v'\,dx \\ &- w^{(3)}(1)v''(1) + w^{(3)}(0)v''(0) + \int_0^1 w^{(3)}v^{(3)}\,dx \\ &+ \int_0^1 wv\,dx + 2\int_0^1 w''v''\,dx \\ =& \int_0^1 w^{(3)}v^{(3)} + 3w''v'' + 3w'v' + wv\,dx \\ =& \langle w, v\rangle_{Z_1}. \end{aligned}$$

Hence, the operator L is symmetric. We prove now that the operator L is bijective. Let us consider first operator

$$L_1 : D(L_1) = \{u \in H^3 : u'(0) = 0, u(1) = 0\} \to H^1, \quad L_1(u) = -u'' + u.$$

From classical results for the mixed boundary value problem (see [Zei90, Theorem 25.I]) there exists a unique solution $u \in H^1$ to the problem $L_1 u = f$, $f \in L^2$ and from the regularity results for solutions of elliptic linear equations it follows that $f \in H^1$ implies $u \in H^3$ and the operator L_1 is bijective.
We study now the operator

$$\begin{aligned} &L_2 : D(L_2) = \{u \in H^5, u'(0) = u'(1) = 0\} \to H^3 \\ &L_2 u = -u'' + u. \end{aligned}$$

From general regularity results for the Laplacian with Neumann boundary conditions (see [Tay96a]) L_2 is bijective. For $L_2 u = f$, $f \in D(L_1)$ implies that $u \in D(L)$ since we can write the boundary conditions as

$$\begin{aligned} (-u'' + u)(1) = f(1) = 0 \\ (-u'' + u)'(0) = f(0) = 0 \end{aligned}$$

and the restriction $L_2 \mid_{D(L)}: D(L) \to D(L_1)$ is bijective. We notice that $L = L_1 \circ L_2 \mid_{D(L)}$ and, as a composition of two bijective functions, L is also bijective. As our operator is symmetric and bijective, it is also self-adjoint (see Lemma 3.9).
Due to Theorem 3.11, L is the Friedrichs extension of the embedding of

$$R(F'(a^\dagger)^*) \hookrightarrow H^1$$

since $R(F'(a^\dagger)^*)$ equipped with the inner product (6.39c) is a Hilbert space, $D(L) = R(F'(a^\dagger)^*)$, and (3.6) is satisfied by virtue of (6.41). Hence, by Remark 3.13 the equality (6.40) holds true. □
It follows from Proposition 6.14 that the Hilbert scale $\{\mathcal{X}_s\}$ generated by the operator $L^{\frac{1}{4}}$ has the desired properties (6.39a), (6.39b) and (6.39c).

Theorem 6.15. *For the Hilbert scale $\{\mathcal{X}_s\}$ defined before and under the supplementary conditions (6.34) and (6.38), Assumption 2 is fulfilled with $p = 2$. Moreover, Assumption 3 is also satisfied under the same conditions if the diameter of $D(F) \cap (a_0 + X_s)$ in X_0-norm is smaller than a $\rho > 0$.*

Proof. By Corollary 3.28 Assumption 2 is equivalent to $\|F'(a^\dagger)^* w\|_{\mathcal{X}_2} \sim \|w\|_{L^2}$ for all $w \in L^2$. The first condition holds true due to (6.39b), and the second due to (6.41) and (6.39c). We check now the Assumption 3, by using again the adjoint of the operator $F'(a^\dagger)^*$(see Lemma 3.5). It follows, by (6.36) that

$$\|(F'(a^\dagger)^* - F'(a)^*)h\|_{\mathcal{X}_2} = \|(\Phi'(a^\dagger(\cdot)) - \Phi'(a(\cdot))) \int_\cdot^1 h(s)\,ds\|_{\mathcal{X}_0}$$
$$\leq \|(\Phi' \circ a^\dagger) - (\Phi' \circ a)\|_{H^1} \| \int_\cdot^1 h(s)\,ds\|_{H^1} \leq c\|a^\dagger - a\|_{\mathcal{X}_0}\|h\|_{L^2}.$$

The last inequality holds because

$$\begin{aligned}
\|(\Phi' \circ a^\dagger) - (\Phi' \circ a)\|_{H^1} =& \|\Phi' \circ a^\dagger - \Phi' \circ a\|_{L^2} + \|(\Phi'' \circ a^\dagger)(a^\dagger)' - (\Phi'' \circ a)a'\|_{L^2} \\
\leq& K\|a^\dagger - a\|_{L^2} + \|(\Phi'' \circ a)((a^\dagger)' - a') \\
&+ (a^\dagger)'(\Phi'' \circ a^\dagger - \Phi'' \circ a))\|_{L^2} \\
\leq& K\|a^\dagger - a\|_{L^2} + K\|(a^\dagger)' - a'\|_{L^2} \\
&+ \|\Phi'' \circ a^\dagger - \Phi'' \circ a\|_\infty \|(a^\dagger)'\|_{L^2} \\
\leq& 2K\|a^\dagger - a\|_{H^1} + \|\Phi''\|_{C^{0,1}}\|a^\dagger - a\|_\infty \|a^\dagger\|_{H^1} \\
\leq& 2K\|a^\dagger - a\|_{H^1} + \|\Phi''\|_{C^{0,1}}\|a^\dagger\|_{H^1}\|a^\dagger - a\|_{H^1}\|a^\dagger\|_{H^1} \\
\leq& C\|a^\dagger - a\|_{H^1}.
\end{aligned}$$

□

Proposition 6.16. *If $a^\dagger \in H^{q+1}$ and $\Phi \in C^{\lceil q \rceil+1,1}$, where $\lceil q \rceil$ is the biggest integer smaller than q, then $u^\dagger \in H^{q+2}$.*

Proof. Since the composition between Φ and $a^\dagger$ belongs to H^{q+1} (see [RR04]), it follows immediately that $u^\dagger \in H^{q+2}$, for $q \geq 2$. □

Now, the optimality follows as in the previous applications:

Theorem 6.17. *In the case of the noise model (2.9), if the assumptions of Theorem 6.15 hold true and if $s \geq 2$, $q \in [s, 2s+2]$, $a^\dagger - a_0 \in \mathcal{X}_q$, and $a^\dagger \in H^{q+1}$, then $u^\dagger$ can be estimated such that (1.5) holds true with $\beta \sim \sigma^{\frac{q+2}{q+2+1/2}}$. Moreover, for the choice $\alpha \sim \sigma^{\frac{2(2+s)}{q+2+1/2}}$ we get*

$$\begin{aligned}
\sqrt{\mathbf{E}\|\widehat{a} - a^\dagger\|_{H^1}^2} &= \mathcal{O}\left(\sigma^{\frac{q}{q+2+1/2}}\right), \\
\sqrt{\mathbf{E}\|\widehat{a} - a^\dagger\|_{L^2}^2} &= \mathcal{O}\left(\sigma^{\frac{q+1}{q+2+1/2}}\right).
\end{aligned}$$

Proof. The first statement follows from Proposition 6.16 and from the theory of nonparametric regression (see [Tsy04]). The second statement is a consequence of Remark 4.7 with $r = 0$ and $r = -1$ and Theorems 6.13 and 6.15. □

Chapter 7

Numerical experiments

In this final chapter we illustrate the influence of the smoothness of the parameter $a^\dagger$ on the rate of convergence of $\widehat{u}$ as shown in Theorem 4.6 by numerical simulation using the application studied in section 6.1. In the first section we review some properties of the local polynomial estimator, method that we use to obtain an estimator $\widehat{u}$ of the exact data $u^\dagger$. Then the second step consists in constructing an estimator for $\widehat{a}$ with the help of the iteratively regularized Gauss-Newton algorithm. The numerical results are discussed in the last section.

7.1 Local polynomial estimator

The first step of our method consists in approximating the data, with the help of a statistical method with known rate of convergence and with known tail-behavior. We are interested in estimating the function $u^\dagger = F(a^\dagger)$ knowing n independent copies of a generic member of the sample (X, Y): $(X_1, Y_1) \cdots (X_n, Y_n)$ where

$$Y_i = u^\dagger(X_i) + \varepsilon_i, \qquad i = 1, .., n.$$

The function

$$u^\dagger(x) = \mathbf{E}(Y|X = x)$$

is the **regression function** of Y over X. The set of values $\{X_1, \ldots, X_n\}$ is called the **design**. This is called **random design** if $\{X_1, \ldots, X_n\}$ are random variables or **fixed design** if they are deterministic values. The direct regression problem to construct an estimator $\widehat{u}$ of $u^\dagger$ from such data and the speed of convergence $\beta \to 0$ as $n \to \infty$ have been studied extensively in the statistical literature (see [Tsy04],[FG96] and references therein).
Here, we choose the local polynomial estimator to solve our direct regression problem. For simplicity we only discuss the case of a univariate function $u^\dagger$.
This method locally fits a polynomial to the data $(Y_i)_{i=1\ldots n}$, using weighted least

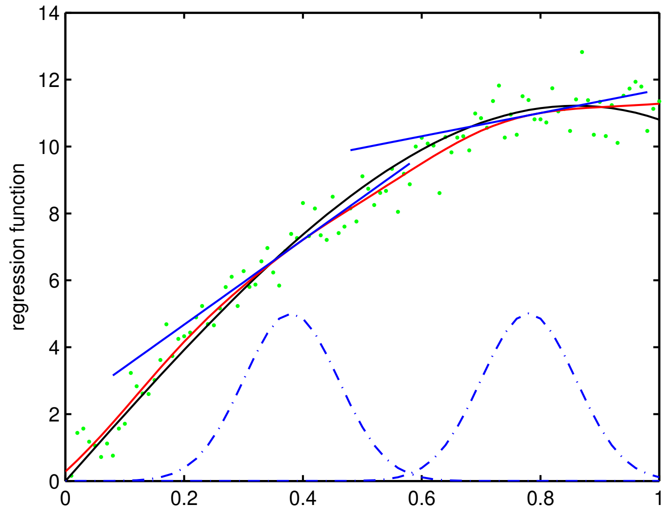

Figure 7.1: Local linear polynomial estimator (red curve) based on 100 simulated observations (green points). The black line is the exact function and the blue lines are the kernel weights and the weighted linear fits at the two points

squares where the weights are chosen according to the height of a kernel function centered about the approximation point (see [FG96, WJ95]). When we perform the local fitting process for every point of the grid, we obtain a curve as in Figure 7.1. For a general polynomial of degree r and a kernel function $K_h(x) = \frac{1}{h}K(\frac{x}{h})$, $K : \mathbf{R} \to [0, \infty)$, $\int_{\mathbf{R}} K = 1$ scaled by a bandwidth h, we obtain the estimator $\widehat{u}(x; r, h)$ in x as the solution of the minimizing problem

$$\min_{\mu \in \mathbf{R}^{r+1}} \sum_{i=1}^{n} \left\{ Y_i - \sum_{k=1}^{r+1} \mu_k (x_i - x)^{k-1} \right\}^2 K_h(x_i - x).$$

We can rewrite this with the help of matrices and vectors

$$X_x = \begin{pmatrix} 1 & x_1 - x & \dots & (x_1 - x)^r \\ 1 & x_2 - x & \dots & (x_2 - x)^r \\ \dots & \dots & \dots & \dots \\ 1 & x_n - x & \dots & (x_n - x)^r \end{pmatrix},$$

$$\begin{aligned} W_x &= \mathbf{diag}\left\{K_h(x_1 - x), \dots, K_h(x_n - x)\right\}, \\ Y &= (Y_1, \dots, Y_n)' \end{aligned}$$

as

$$\widehat{u}(x; r, h) = \left(X_x' W_x X_x\right)^{-1} X_x' W_x Y \tag{7.1}$$

if the matrix $X_x' W_x X_x$ is invertible.
The choice of the bandwidth parameter h is fundamental for the quality of the estimator. The weight assigned to a particular point Y_i is $K_h(X_i - x)$, which means that, for a usual kernel shape, the observations close to x have more influence on the regression estimate at x than those farther away. The bandwidth h controls the amount of the relative influence of the observations, for a small h the estimator value depends heavily on the closest observations, for $h \to 0$ the estimator tends to interpolate the data and for a large h the estimates tends to the least square estimator of the data (see [FG96]).
We consider a fixed design in our numerical simulations and, from the convergence analysis in [Tsy04], it follows that, for an a-priori choice of the bandwidth h of order $n^{-\frac{1}{2q+1}}$, the quadratic risk is order-optimal

$$\mathbf{E}\|\widehat{u} - u^\dagger\|_{L^2}^2 = \mathcal{O}\left(n^{\frac{-2q}{2q+1}}\right).$$

if $u^\dagger$ belongs to the Sobolev space H^q.

7.2 Minimization of the Tikhonov functional

To minimiza the tikhonov functional global results were obtained by Ramlau and others [Ram03, RT05, LPR07] under certain conditions. These algorithms start with a large regularization parameter and decrease it gradually to the desired value.
We used a Levenberg-Marquardt type algorithm to minimize the Tikhonov functional (4.2), which reduces to the iterated regularized Gauss-Newton method (1.4b) with constant regularization parameter $\alpha_k = \alpha$. Even though this method certainly converges only locally in general, we did not observe any convergence problems for the example studied in the following section.
In the k-th iteration step we have to solve the least-squares problem

$$\min_{h \in \mathcal{X}_s} \|T_k h - b_k\|_{\mathcal{Y} \oplus \mathcal{X}_s} \tag{7.2}$$

for the update $h_k = a_{k+1} - a_k$, where the right hand side $b_k \in \mathcal{Z} = \mathcal{Y} \oplus \mathcal{X}_s$ and the linear operator $T_k : \mathcal{X}_s \to \mathcal{Z}$ are defined by

$$T_k = \begin{pmatrix} F'(a_k) \\ \sqrt{\alpha_k} I \end{pmatrix}$$

and

$$b_k = \begin{pmatrix} \widehat{u} - F(a_k) \\ \sqrt{\alpha}(a_0 - a_k) \end{pmatrix}.$$

To avoid setting up the entire matrix representing T_k in a discrete setting , we solve (7.2) by the conjugate gradient method applied to the normal equation

$$T_k^* T_k h = T_k^* b_k. \tag{7.3}$$

For the examples discussed in the sections 6.1 and 6.2, the computation of a matrix-vector product with T_k involves the solution of an elliptic boundary value problem, for the example in section 6.3 the evaluation of the adjoint T_k^* is not always as straightforward due to the choice of the Hilbert scales $\mathcal{X}_s$.
We consider now more generally the situation that we want to solve a normal equation

$$\tilde{T}^* \tilde{T} h = \tilde{T}^* b \tag{7.4}$$

with a linear bounded operator $\tilde{T} : \tilde{\mathcal{X}} \to \tilde{\mathcal{Z}}$ and that we have at our disposal only the adjoint of the extension $T : \mathcal{X} \to \mathcal{Z}$ of $\tilde{T}$ where $\tilde{\mathcal{X}} \subseteq \mathcal{X}$, $\tilde{\mathcal{Z}} \subseteq \mathcal{Z}$ are dense subspaces and $\tilde{T}x = Tx$ for all $x \in \tilde{X}$. The norms of $\tilde{\mathcal{X}}$ and $\tilde{\mathcal{Z}}$ are given in terms of self-adjoint operators $L_\mathcal{X} : \tilde{\mathcal{X}} \to \mathcal{X}$ and $L_\mathcal{Z} : \tilde{\mathcal{Z}} \to \mathcal{Z}$

$$\|x\|_{\tilde{\mathcal{X}}} = \|L_\mathcal{X} x\|_\mathcal{X} \qquad \|z\|_{\tilde{\mathcal{Z}}} = \|L_\mathcal{Z} z\|_\mathcal{Z}.$$

Then we have

$$\tilde{T}^* = L_\mathcal{X}^{-2} T^* L_\mathcal{Z}^2.$$

In sections 6.1 and 6.2 the Hilbert scales are generated by square roots of differential operators. Therefore, $L_\mathcal{X}$ and $L_\mathcal{Z}$ are difficult to represent numerically if s is an odd integer, but $L_\mathcal{X}^2$ and $L_\mathcal{Z}^2$ are easy to represent. A similar situation arises in example in section 6.3 if $\frac{s}{2}$ is an odd integer since the Hilbert scale is generated by the fourth root of fourth order differential operator. The following conjugate gradient algorithm solves the normal equation (7.4) accessing only matrix vector products, the operator $G_\mathcal{Z} := L_\mathcal{Z}^2$, the inverse of the operator $G_\mathcal{X} = L_\mathcal{X}^2$, T_k and T_k^* (see [Han95, GHO99]). In a discrete setting, the operator $G_\mathcal{X}$ and $G_\mathcal{Z}$ are represented by the Gram matrices with respect to the chosen basis. We solve the normal equation (7.3) corresponding to the k-th step of the Levenberg-Marquardt algorithm with operator T_k, right hand side b_k and unknown h_k. The initial value for h_k is chosen, for simplicity, $h_k^0 = 0$. In the l-th step of the CG- algorithm we compute the residual r^l, the search direction d^l, the auxiliary parameters $\tilde{r}^l$, f^l, $\tilde{f}^l$, α^l and β^l. Here the parameter $\rho > 0$ in the stopping criterion determines the accuracy of the result. We always choose $\rho = 0.001$.

Algorithm 7.1 (Conjugate Gradient Algorithm)**.**

$$
\begin{aligned}
&h_k^{(0)} = 0; s^{(0)} = b_k - T_k h_k^{(0)}; \tilde{s}^{(0)} = G_{\mathcal{Z}} s^{(0)};\\
&\tilde{r}^{(0)} = T_k^* \tilde{s}^{(0)}; r^{(0)} = G_{\mathcal{X}}^{-1} \tilde{r}^{(0)}; d^{(0)} = r^{(0)}; l = 0;\\
&\text{while}(\left\langle \tilde{s}^{(l)}, s^{(l)} \right\rangle_{\mathcal{Z}} > \rho^2 \left\langle \tilde{s}^{(0)}, s^{(0)} \right\rangle_{Z})\\
&\quad l = l + 1;\\
&\quad f^{(l)} = T_k d^{(l)};\\
&\quad \tilde{f}^{(l)} = G_{\mathcal{Z}} f^{(l)};\\
&\quad \alpha^{(l)} = \frac{\left\langle r^{(l)}, \tilde{r}^{(l)} \right\rangle_{\mathcal{X}}}{\left\langle f^{(l)}, \tilde{f}^{(l)} \right\rangle_{Z}};\\
&\quad h_k^{(l)} = h_k^{(l-1)} + \alpha^{(l)} d^{(l-1)};\\
&\quad s^{(l)} = s^{(l-1)} - \alpha^{(l)} \tilde{f}^{(l)};\\
&\quad \tilde{r}^{(l)} = T_k^* \tilde{s}^{(l)};\\
&\quad r^{(l)} = G_{\mathcal{X}}^{-1} \tilde{r}^{(l)};\\
&\quad \beta^{(l)} = \frac{\left\langle r^{(l)}, \tilde{r}^{(l)} \right\rangle_{\mathcal{X}}}{\left\langle r^{(l-1)}, \tilde{r}^{(l-1)} \right\rangle_{\mathcal{X}}};\\
&\quad d^{(l)} = r^{(l)} + \beta^{(l)} d^{(l-1)};
\end{aligned}
$$

7.3 Numerical simulations

In our numerical simulations, we construct $\widehat{a}$ starting from $\widehat{u}$ by Tikhonov regularization in Hilbert scales as the solution of the minimization problem (7.3). We consider the parameter-to-solution operator F like in Application 6.3, the domain $\Omega = (0,1)$ and we choose the Hilbert scale $\{X_t\}_{t\in\mathbf{R}}$ generated by the operator $T(1)$ defined in Example 3.19. Hence, we have

$$\mathcal{X}_0 = L^2, \quad \mathcal{X}_2 = H_2 \cap H_0^1$$

We assume that the exact solution $a^\dagger$ is in $\mathcal{X}_q$ and we choose an index $s \in [\frac{q-2}{2}, q]$ for the penalization norm, since the ill-posedness of the problem is $p = 2$. Since in our simulation we choose $s = 2$, the norm $\|\cdot\|_{\mathcal{X}_s}$ is the $\|\cdot\|_{H^2}$-norm on $\mathcal{X}_2 = H_2 \cap H_0^1$. Due to Poincaré lemma, the norm on $\mathcal{X}_2$, is equivalent to

$$\|u\|_{\mathcal{X}_2} \sim \|u''\|_{L^2}.$$

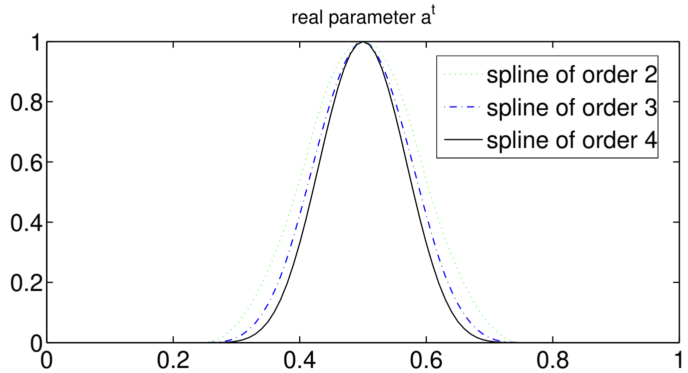

Figure 7.2: Parameter functions $a^\dagger$ with different degrees of smoothness used in the tests

Numerically, we compute the Laplacian $\bigtriangledown^2$ with the help of finite differences matrix K

$$K = m^2 \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 \\ \dots & \dots & \dots & \dots & & \\ 0 & 0 & 0 & 0 & \dots & 1 \end{pmatrix},$$

and we use this matrix to compute the norms $\|u''\|_{L^2}$ and the solution of the direct problem $F(a) = u$. As we already saw in Remark 6.1 we need the knowledge of the boundary conditions of the reaction term $a^\dagger$ to be able to identify it, knowledge expressed with the help of the initial guess $a_0 = 0$ in this case. In our example we choose the function to estimate $a^\dagger$

$$a^\dagger(x) = x - x^2 + B_p(2(p+1)(x - \frac{1}{2})) \tag{7.5}$$

where the functions B_p are the B-splines of order p defined recursively

$$B_0(x) = \begin{cases} 1, & |x| < \frac{1}{2} \\ 0, & \text{otherwise} \end{cases}$$

$$B_{p+1}(x) = \int_{x-\frac{1}{2}}^{x+\frac{1}{2}} B_p(t)\,dt,\ m = 0, 1 \dots .$$

Since the B-splines of order 2, 3 or 4 correspond to smoothness up to $H^{2.5}$, $H^{3.5}$ and $H^{4.5}$ respectively (as the splines of order q belong to the intersection of H^r spaces with $0 < r < q$) with zero boundary conditions, we consider the smoothness q equal to $2, 3$ and respectively 4. Figure 7.2 presents the three different choices of the true parameter $a^\dagger$.

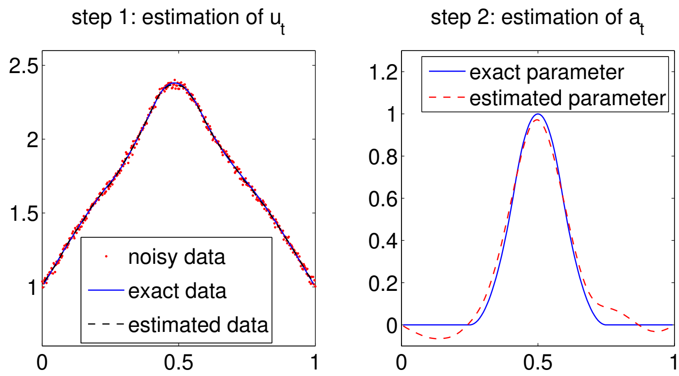

Figure 7.3: Illustration of the method for the spline of order 2 and simulated data with 1% noise. Left: step 1, estimation of the solution $u^\dagger$ to the differential equation, Right: step 2, estimation of the unknown parameter $a^\dagger$.

The direct problem is solved by finite differences, on an equidistant grid. Details of finite differences can be found, for example, in [Hac92]. We assume an equally spaced deterministic design regression problem and we generate our data $(Y_i)_{i=1\dots n}$ as

$$Y_i = u^\dagger(x_i) + \sigma\epsilon_i,\ i = 1\dots n$$

where $x_i = \frac{i}{n}$, ϵ_i are independent, $N(0,1)$, random variables and the noise level is $\sigma = 0.01$. Since we study asymptotical behavior, we choose the sample sizes $n = 398, 1000, 2512, 6310, 15849, 39811, 100000$ and 251189 respectively. Fig. 7.3 shows the exact data $u^\dagger$ and the noisy data with 1% noise for a data sample of size 381 if $a^\dagger$ is a spline of order two.
We estimate $u^\dagger$ on an equidistant grid with $m = 100$ points in $[0,1]$. Since $u^\dagger$ belongs at least to the Sobolev space H^{q+2}, which is continuously embedded in C^{q+1}, we can approximate it by a polynomial of order up to $q+1$. As we saw, the choice of the bandwidth of order $n^{\frac{-1}{2r+3}}$ is asymptotically optimal and we used this a-priori choice of h in our applications (see e.g. [FG96]). We choose the Gaussian kernel $K_h(t) = \frac{1}{\sqrt{2\pi h^2}}\exp(\frac{-t^2}{2h^2})$ and the local polynomial estimator of order 5, since this insures the optimal rates for smoothness of order 6 and since an odd order is advisable as the variability increases when passing from an odd order of the polynomial to an even one and it does not vary when going from an even to an odd order.

We chose the H^2-norm for the regularization term in the Tikhonov functional so $s = 2$, $p = 2$ and $q \approx 2.5, 3.5$, and 4.5, respectively.
The convergence rates for our method are illustrated in Fig. 7.4, considering different sample sizes n and 200 simulations for each sample size. We plot the

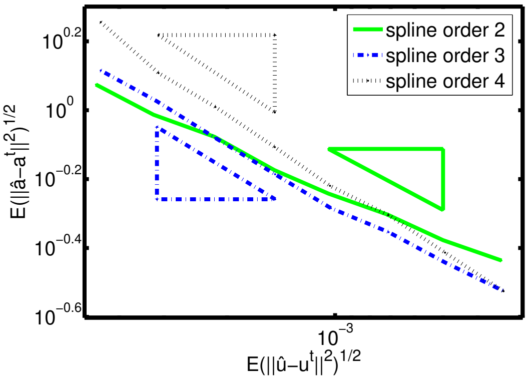

Figure 7.4: Convergence plots for the parameter functions shown in Fig. 7.2. The triangles indicate the slopes predicted by Theorem 4.6.

empirical estimation of the expected square error of $\widehat{a}$ over the empirical estimation of the square error of $\widehat{u}$ for the three choices of $a^{\dagger}$ shown in Fig. 7.2. On both axes a logarithmic scale is used such that according to Theorem 4.6 the plot are expected to be straight lines. The slopes of these straight lines predicted from Theorem 4.6 are indicated by triangles. The empirical slopes of the convergence plots are indeed close to the predicted slopes.

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