Iterative Methods in Inverse Obstacle Scattering: Regularization Theory of Linear and Nonlinear Exponentially Ill-Posed Problems

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Contents

0. Introduction

Abstract

Our investigations are motivated by the classical inverse scattering problems to reconstruct the shape of impenetrable obstacles from far field measurements of scattered time-harmonic acoustic or electromagnetic waves in the resonance region. These problems, which are nonlinear and exponentially ill-posed, can be tackled quite successfully by iterative regularization methods, in particular regularized Newton methods. We give, for the first time, convergence and convergence rate results for such methods. These results are also applicable to a number of exponentially ill-posed problems in inverse heat conduction, satellite gradiometry, and potential theory.

In the first part of this work we look at derivatives of the scattered field with respect to the shape of the scattering obstacle. We show that the field depends analytically on the shape of the obstacle and give a characterization of derivatives of arbitrary order. Based on these results we describe an efficient implementation of the derivatives. In the second part, we first study regularization theory for linear exponentially ill-posed problems. Then we look at the speed of convergence of iterative regularization methods, in particular regularized Newton methods in inverse obstacle scattering. As a consequence of the severe ill-posedness, standard Hölder-type source conditions, which yield convergence rates in form of fractional powers of the data noise level, are far too restrictive for inverse obstacle scattering problems. We introduce a weaker type of source conditions that imply convergence rates which are only logarithmic in the data noise level and show that these conditions are natural in the sense that they are essentially equivalent to smoothness and closeness conditions for the difference between the initial guess and the exact solution in terms of Sobolev spaces. These results are confirmed in numerical experiments.

Let us start with a brief description of the physical background that leads to the mathematical formulation of direct and inverse scattering problems.

We consider a compact set $K \subset \mathbb{R}^m$, $m \in \{2,3\}$ describing the scattering obstacle. The case $m = 2$ corresponds to scattering by long cylinders. It is well known that the propagation of an acoustic wave in a homogeneous, isotropic and inviscid fluid can approximately be described by a *velocity potential* $U(x,t)$ satisfying the wave equation

$$\frac{1}{c^2}\frac{\partial^2 U}{\partial t^2} = \Delta U.$$

Here c is the speed of sound, $v = \operatorname{grad}_x U$ is the velocity field, and $p = -\frac{\partial U}{\partial t}$ is the pressure. For more information on the physical background leading to this equation we refer, e.g., to Colton and Kress [CK97] or Werner [Wer61].

If U is time-harmonic, i.e.

$$U(x,t) = \operatorname{Re}\left(u(x)\mathrm{e}^{-\mathrm{i}\omega t}\right), \qquad \omega > 0$$

in complex notation, then the complex-valued space-dependent part u satisfies the *Helmholtz equation*

$$\Delta u + \kappa^2 u = 0 \quad \text{in } \mathbb{R}^m \backslash K. \tag{0.1}$$

Here $\kappa = \omega/c$ is the *wave number*. Moreover, the total field u satisfies some boundary condition at ∂K depending on the physical properties of the surface. E.g., for "sound-soft" obstacles the pressure p vanishes on ∂K, so u satisfies the Dirichlet boundary condition

$$u = 0 \qquad \text{on } \partial K. \tag{0.2}$$

Similarly, for "sound-hard" obstacles the normal component $\langle \nu, v\rangle$ of the velocity v vanishes, so we get the Neumann boundary condition

$$\frac{\partial u}{\partial \nu} = 0 \qquad \text{on } \partial K. \tag{0.3}$$

(ν denotes the exterior normal vector on ∂K.) We will consider the situation that $u = u_\mathrm{i} + u_\mathrm{s}$ is composed of a known incident wave u_i, typically a plane wave $u_\mathrm{i}(x) = e^{i\kappa\langle d,x\rangle}$ with direction d, $|d| = 1$, and a scattered wave u_s. The scattered field additionally satisfies the *Sommerfeld radiation condition*

$$\lim_{r\to\infty} r^{\frac{m-1}{2}} \left\{ \frac{\partial u_\mathrm{s}}{\partial r} - i\kappa u_\mathrm{s} \right\} = 0, \qquad r = |x|. \tag{0.4}$$

Physically, this condition means that energy is carried away from the scatterer, and mathematically it ensures uniqueness of the solution to the scattering problem. It can be shown that (0.4) implies the asymptotic behavior

$$u_\mathrm{s}(x) = \frac{e^{i\kappa|x|}}{|x|^{\frac{m-1}{2}}} \left\{ u_\infty\left(\frac{x}{|x|}\right) + \mathrm{O}\left(\frac{1}{|x|}\right)\right\}, \qquad |x| \to \infty. \tag{0.5}$$

A function which satisfies (0.1) and (0.4) is called a *radiating solution* to the Helmholtz equation. The function $u_\infty : \{x : |x| = 1\} \to \mathbb{C}$ is called the *far field pattern* or *scattering amplitude*. It is always an analytic function (cf. [CK97]).

The *direct scattering problem* consists in finding $u_{\rm s}$ as solution to the exterior boundary value problem (0.1), (0.4) with one of the boundary conditions (0.2) or (0.3), given $u_{\rm i}$ and K. This problem is well understood. We are interested in the *inverse problem* to find an approximation to K, given $u_{\rm i}$ and measurement data u_∞^δ of the exact far field pattern u_∞. Here δ denotes the noise level, which is usually measured in the L^2-norm, i.e. $\|u_\infty^\delta - u_\infty\| \le \delta$. Let the set of admissible scatterers K be described by an open subset $D(F)$ of a Hilbert space X, e.g. a Sobolev space of parametrizations. Let us introduce the operator $F : D(F) \to L^2(S^{m-1})$ that maps a description $q \in D(F)$ of some admissible scatterer K to to the corresponding far field pattern $u_\infty \in L^2(S^{m-1})$. Then the inverse scattering problem described above can be formulated as a nonlinear operator equation

$$F(q) = u_\infty^\delta. \tag{0.6}$$

This problem is ill-posed in the sense that $F^{-1} : R(F) \to D(F)$ (if it exists) is not continuous for any reasonable norm in X. (Note that we are *not* free to choose the norm in the image space since it has to describe the measurement errors!) The ill-posedness follows from the fact that F is locally compact (e.g. from C^1 to L^2, cf. [CK97, Theorem 5.9]). The fact that F maps an arbitrary $q \in D(F)$ to an analytic function u_∞ is an indication that (0.6) is *severely ill-posed*. Another indication is that the singular values of $F'[q]$ decay like $\frac{1}{n!}$, i.e. slightly faster than exponentially. This means that the data noise error for the nth singular vector is amplified by a factor proportional to $n!$. Therefore, the effects of data noise or computational errors will be disastrous unless some regularization techniques are employed.

One class of methods (e.g. the Colton-Monk, Kirsch-Kreß, or AKR-methods, cf. [CM85a, CM85b, KK87a, KK87b, AKR87, KKMZ88, CK97]) consists in splitting the inverse scattering problem into the ill-posed, but linear problem to reconstruct u_s from u_∞ and the nonlinear, but usually well-posed problem to find ∂K from the boundary condition (0.2) or (0.3) for the total field. An advantage of this class of methods is that costly evaluations of the operator F and its derivatives are avoided.

Another class of methods has recently been introduced by Colton, Kirsch, Potthast and others (cf. [CK96, Pot96a, CPP97, Kir98]). These methods do not require any a-priori knowledge about the topology of the scatterer (e.g. the number of connectivity components or the gender of the surfaces) or of the type of boundary condition. Therefore, these methods can be used to provide a good initial guess for iterative methods. As an example we briefly describe the method in [Kir98]. The starting point is the observation that a point $x \in \mathbb{R}^m$ belongs to the interior of K if and only if the far field pattern $\exp(-i\kappa \langle \cdot, x\rangle)$ of the point source at x belongs to the range of the operator A which maps a function on ∂K to the far field pattern of the solution to the corresponding boundary value problem. It is shown that $\operatorname{ran}(A) = \operatorname{ran}((\mathcal{F}^*\mathcal{F})^{\frac{1}{4}})$ where $\mathcal{F}$ is the integral operator with kernel $u_\infty(\hat{x}, d)$. This gives a simple characterization of K by $u_\infty(\hat{x}, d)$ which leads to a numerical algorithm to reconstruct K approximately from $u_\infty(\hat{x}, d)$. Note that this method requires far field data of incident waves for *all* directions d.

Finally, iterative regularization methods have been studied intensively over the last years both in an abstract setting and for inverse scattering as well as many other problems. These methods, in particular regularized Newton methods, tend to yield more accurate reconstructions than the other methods. (We refer to [Kre97] for a comparison with the first class of methods.) In all of these methods the operator F has to be evaluated in each iteration step, and usually also the Fréchet derivative $F'[q]$ or its adjoint $F'[q]^*$. Some methods suggested by Hettlich and Rundell also use the second Fréchet derivative $F''[q]$ of F.

Although iterative methods have been used successfully before, there has been a lack of convergence results. It is the purpose of this work to provide such results, and in particular estimates on the speed of convergence. According to a well-known result convergence of any regularization method for an ill-posed problem can be arbitrarily slow without a-priori information (cf. [EHN96, Proposition 3.11.]). In standard regularization theory such a-priori information are provided in form of Hölder-type source conditions. For nonlinear problems such conditions have the form

$$q_0 - q^\dagger = (F'[q^\dagger]^* F'[q^\dagger])^\mu w, \qquad \mu > 0,$$

where q_0 is an initial guess and $q^\dagger$ is the exact solution. Such conditions are far too restrictive for exponentially ill-posed problems. Appropriate conditions turn out to be of the form

$$q_0 - q^\dagger = (-\ln F'[q^\dagger]^* F'[q^\dagger])^{-p} w, \qquad p > 0. \tag{0.7}$$

For many linear and nonlinear exponentially ill-posed problems such so-called *logarithmic source conditions* can be interpreted as smoothness conditions for the initial error $q_0 - q^\dagger$ in terms of Sobolev spaces.

We first study the convergence of standard regularization methods for *linear problems* under logarithmic source conditions. Whereas Hölder-type source conditions imply convergence rates of the order $\mathrm{O}\left(\delta^{\frac{2\mu}{2\mu+1}}\right)$, the best possible order of convergence that can be obtained under logarithmic source conditions is of the order $\mathrm{O}\left((-\ln\delta)^{-p}\right)$ which is much slower. We introduce an a-posteriori parameter choice rule leading to *asymptotically* optimal convergence. Moreover, we look at the influence of operator approximations in such situations. Then we turn our attention to nonlinear problems and show that under assumption (0.7), some condition restricting the degree of nonlinearity of F, and under a closeness condition the iteratively regularized Gauß-Newton method converges of optimal order $\|q^\dagger - q_N^\delta\| = \mathrm{O}\left((-\ln\delta)^{-p}\right)$. Here N denotes the stopping index, and q_N^δ is the final iterate. For exact data, we get $\|q^\dagger - q_n\| = \mathrm{O}\left(n^{-p}\right)$ as $n \to \infty$.

This thesis is divided into 5 chapters. The first chapter is concerned with Fréchet derivatives of F. We show that F is analytic, even for rough boundaries, and give a characterization of Fréchet derivatives of arbitrary order. Chapter 2 is devoted to efficient numerical implementations of Fréchet derivatives. In Chapter 3 we develop a regularization theory for linear problems under logarithmic source conditions and give some applications to inverse problems in heat conduction and satellite gradiometry. Chapter 4 is concerned with *nonlinear* exponentially ill-posed problems with particular emphasis on inverse scattering problems. Finally, in Chapter 5 we report on numerical experiments which confirm our theoretical results.

1. Derivatives with respect to the domain

In this chapter we look at the total field u as a function of the obstacle K and describe derivatives of u with respect to K. These derivatives are needed for iterative regularization methods for inverse scattering problems. Therefore, over the last years a lot of effort has been spent to characterize and to compute Fréchet derivatives of scattering problems (cf. [Het95, Het98, HR, Kir93, Kre94, Kre95a, Kre95b, Mön96, Mön97, Pot94, Pot96b]). Here, we present a new approach that combines techniques from [Kir93] and [Sim80] with some new ideas, and yields a simplification and improvement of existing results. We show that u depends *analytically* on K even if K is rough. Here domains are described by differentiable functions on a reference domain. Moreover, we compute the boundary values of the derivatives of u of *arbitrary order* on smooth parts of ∂K.

We mention that analytic dependence of u on K has been used successfully to compute u numerically by Taylor or Padé approximation for domains K that are close to some simple shape (cf. Gosh Roy et al. [RCW97, RWCS98]). The results below provide a theoretical foundation for these methods.

1.1. Dirichlet boundary conditions

1.1.1. The sound-soft scattering problem

Assume that $K \subset \mathbb{R}^m$, $m \in \{2, 3\}$, is compact and that ${}^cK := \mathbb{R}^m \backslash K$ is connected. We do not require any smoothness but closedness in the sound-soft case. First, we define what is meant by a solution to the sound-soft scattering problem for such general domains, and then establish existence and uniqueness.

Choose $R > 0$ such that $K \subset \{x \in \mathbb{R}^m : |x| < R\}$, and set $\Omega_R := \{x \in {}^cK : |x| < R\}$ and $S_R := \{x \in \mathbb{R}^m : |x| = R\}$. We introduce the Sobolev norm

$$\|v\|_{W^1(\Omega_R)} := \left(\int_{\Omega_R} (|v|^2 + |\nabla v|^2) \, dx \right)^{\frac{1}{2}},$$

and define the Sobolev space $W^1_{0,\partial K}(\Omega_R)$ to be the completion under the norm $\|\cdot\|_{W^1}$ of the space of function $v \in C^\infty(\Omega_R)$ that satisfy $\|v\|_{W^1} < \infty$ and vanish in a neighborhood of K.

Problem 1.1. Let $u_\mathrm{i} \in C^2(\mathbb{R}^m)$ be an incident field solving the Helmholz equation $\Delta u_\mathrm{i} + \kappa^2 u_\mathrm{i} = 0$ in $\mathbb{R}^m$. A function $u_\mathrm{s} \in C^2({}^c K)$ is called a *solution to the sound-soft scattering problem* for u_i if (0.1) and (0.4) hold, and (0.2) is satisfied in the sense that

$$u|_{\Omega_R} \in W^1_{0,\partial K}(\Omega_R).$$

To establish existence and uniqueness of a solution, we follow an approach by Kress and Zinn. The problem is transformed to a variational problem on the bounded domain Ω_R, and the radiation condition is incorporated as a nonlocal boundary condition on S_R involving the Dirichlet-to-Neumann map $L : W^{1/2}(S_R) \to W^{-1/2}(S_R)$. L maps a function $f \in W^{1/2}(S_R)$ to the Neumann boundary values $\frac{\partial w}{\partial \nu}|_{S_R}$ of the radiating solution w to the Helmholtz equation with Dirichlet boundary values f. For a different approach based on the limiting absorption principle we refer to Taylor [Tay96, §9.12].

Lemma 1.1. (Variational formulation) *Define the sesquilinear form $S : W^1_{0,\partial K}(\Omega_R) \times W^1_{0,\partial K}(\Omega_R) \to \mathbb{C}$ and the antilinear functional $F \in W^1_{0,\partial K}(\Omega_R)'$ as follows:*

$$S(u,v) := \int_{\Omega_R} \left\{ \nabla u \nabla \bar{v} - \kappa^2 u \bar{v} \right\} dx - \int_{S_R} L u \, \bar{v} \, ds, \tag{1.1}$$

$$F(v) := \int_{S_R} \left\{ \frac{\partial u_\mathrm{i}}{\partial \nu} - L u_\mathrm{i} \right\} \bar{v} \, ds. \tag{1.2}$$

If u is a solution to the sound-soft scattering problem then the variational equation

$$S(u|_{\Omega_R}, v) = F(v) \qquad \text{for all } v \in W^1_{0,\partial K}(\Omega_R) \tag{1.3}$$

holds. Vice versa, if (1.3) is satisfied for some $u \in W^1_{0,\partial K}(\Omega_R)$, then there is an extension of u from Ω_R to ${}^cK$ that solves the sound-soft scattering problem.

Proof. Let u be a solution to the sound-soft scattering problem. From the definition of $W^1_{0,\partial K}(\Omega_R)$ it follows by an approximation argument that Green's formula in $\{x \in \mathbb{R}^m : |x| < R\}$ holds for u and any $v \in W^1_{0,\partial K}(\Omega_R)$ if we extend u and v on K by 0. We obtain

$$\int_{\Omega_R} \left\{ \nabla u \nabla \bar{v} - \kappa^2 u \bar{v} \right\} \, \mathrm{d}x = \int_{S_R} \frac{\partial u}{\partial \nu} \bar{v} \, \mathrm{d}s.$$

This implies (1.3) since $\frac{\partial u}{\partial \nu}\big|_- = \frac{\partial u_{\mathrm{i}}}{\partial \nu} + L(u|_- - u_{\mathrm{i}})$. (Here and in the following, the subscripts $+$, $-$ refer to limits from the exterior and interior of S_R, rsp.)

Now assume that $u \in W^1_{0,\partial K}(\Omega_R)$ solves (1.3). Then, by standard interior regularity results for elliptic boundary value problems, $u \in C^2(\Omega_R)$ and $\Delta u + \kappa^2 u = 0$ in Ω_R. We extend $u_{\mathrm{s}} := u - u_{\mathrm{i}}$ to $\{x \in \mathbb{R}^m : |x| > R\}$ as a radiating solution to the Helmholtz equation satisfying $u_{\mathrm{s}}|_+ = u_{\mathrm{s}}|_-$ on S_R. By (1.3), u satisfies the Neumann condition $\frac{\partial u}{\partial \nu}\big|_- = Lu|_- + \frac{\partial u_{\mathrm{i}}}{\partial \nu} - Lu_{\mathrm{i}}$, i.e. $\frac{\partial u_{\mathrm{s}}}{\partial \nu}\big|_- = Lu_{\mathrm{s}}|_- = \frac{\partial u_{\mathrm{s}}}{\partial \nu}\big|_+$. From the identical Cauchy data of u_{s} on both sides of S_R, we conclude that $u_{\mathrm{s}} \in C^2({}^cK)$ and that (0.1) holds. ■

We need the following properties of the Dirichlet-to-Neumann map on S_R:

Lemma 1.2. *1. There exists a compact linear operator $\tilde{L} : W^{1/2}(S_R) \to W^{-1/2}(S_R)$ such that*

$$\operatorname{Re} \left\langle (-L + \tilde{L})w, w \right\rangle \geq 0 \tag{1.4}$$

for $w \in W^{1/2}(S_R)$.

2. $\operatorname{Im} \langle Lw, w \rangle \leq 0$ for $w \in W^{1/2}(S_R)$ implies $w = 0$.

Proof. The proof for $m = 3$ is given in [CK97, p. 116ff.]. Here we only consider the case $m = 2$, using a similar argument. Let $v_n(R\cos t, R\sin t) := e^{int}$, $n \in \mathbb{Z}$ be the trigonometric monomials on S_R. Then it is easily seen by separation of variables in polar coordinates that

$$Lw = \sum_{n \in \mathbb{Z}} \gamma_n w_n v_n, \qquad \gamma_n := \kappa \frac{H^{(1)\prime}_{|n|}(\kappa R)}{H^{(1)}_{|n|}(\kappa R)}.$$

for $w = \sum_{n \in \mathbb{Z}} w_n v_n$. Here $H^{(1)}_{|n|}$ is the Hankel function of the first kind of order $|n|$. From the formula $H^{(1)\prime}_n(t) = -\frac{n}{t} H^{(1)}_n(t) + H^{(1)}_{n-1}(t)$, $n \geq 1$, we obtain

$$\gamma_n = -\frac{|n|}{R} + \kappa \frac{H^{(1)}_{|n|-1}(\kappa R)}{H^{(1)}_{|n|}(\kappa R)}, \qquad n \neq 0,$$

and the asymptotic formula

$$H_n^{(1)}(t) = \frac{2^n(n-1)!}{\pi i t^n}\left(1 + \mathrm{O}\left(\frac{1}{n}\right)\right), \qquad n \to \infty \tag{1.5}$$

(cf. [CK97, (3.58)]) yields

$$\kappa \frac{H_{|n|-1}^{(1)}(t)}{H_{|n|}^{(1)}(t)} = \frac{t}{2(|n|-1)}\left(1 + O\left(\frac{1}{|n|}\right)\right), \qquad |n| \to \infty. \tag{1.6}$$

We now define

$$\tilde{L} v_n := \kappa \frac{H_{|n|-1}^{(1)}(\kappa R)}{H_{|n|-1}^{(1)}(\kappa R)} v_n.$$

From $\|w\|^2_{W^p(S_R)} = \sum_{n\in\mathbb{Z}}(1+n^2)^p|w_n|^2$, $p \in \mathbb{R}$ and (1.6), it follows that $\tilde{L}$ is a norm limit of finite rank operators, and therefore compact. Moreover,

$$\mathrm{Re}\left\langle(-L+\tilde{L})w, w\right\rangle = \frac{1}{R}\sum_{n\in\mathbb{Z}}|n||w_n|^2 \geq 0.$$

To show the second assertion, we need the formula

$$\mathrm{Im}\,\langle Lw, w\rangle = \sum_{n\in\mathbb{Z}} \mathrm{Im}\,\gamma_n |w_n|^2$$

with

$$\mathrm{Im}\,\gamma_n = \frac{\kappa}{|H_{|n|}^{(1)}(\kappa R)|^2}\det\begin{pmatrix} \mathrm{Re}\,H_{|n|}^{(1)}(\kappa R) & \mathrm{Im}\,H_{|n|}^{(1)}(\kappa R) \\ \mathrm{Re}\,H_{|n|}^{(1)\prime}(\kappa R) & \mathrm{Im}\,H_{|n|}^{(1)\prime}(\kappa R)\end{pmatrix}.$$

Here the determinant is the Wronskian of the Bessel differential equation, which is $\frac{2}{\pi\kappa R}$ (cf. [CK97, p.65]). Thus $\mathrm{Im}\,\gamma_n \geq 0$, and the assertion follows. ■

The following result is given in a similar form in [CK97, Theorem 5.7].

Theorem 1.3. *The operator* $A : W^1_{0,\partial K}(\Omega_R) \to W^1_{0,\partial K}(\Omega_R)'$ *defined by the sesquilinear form* S,

$$S(u, v) = \langle Au, v\rangle_{L^2(\Omega_R)} \qquad u, v \in W^1_{0,\partial K}(\Omega_R), \tag{1.7}$$

is bounded and boundedly invertible. Consequently, the sound-soft scattering problem has the unique solution $u = A^{-1}F$.

Proof. By virtue of (1.4), we have the Gårding-type inequality

$$\operatorname{Re}\left\{S(w,w)+(\kappa^2+1)(w,w)_{L^2(\Omega_R)}+\left\langle \tilde{L}\operatorname{Tr}w,\operatorname{Tr}w\right\rangle_{L^2(S_R)}\right\}\geq \|w\|^2_{W^1_{0,\partial K}(\Omega_R)}$$

with the trace operator $\operatorname{Tr}: W^1_{0,\partial K}(\Omega_R)\to W^{1/2}(S_R)$. It follows from the Lax-Milgram Theorem that the operator

$$A+(\kappa^2+1)\iota+\operatorname{Tr}'\tilde{L}\operatorname{Tr}: W^1_{0,\partial K}(\Omega_R)\to W^1_{0,\partial K}(\Omega_R)'$$

has a bounded inverse. Since the embedding $\iota: W^1_{0,\partial K}(\Omega_R)\hookrightarrow W^1_{0,\partial K}(\Omega_R)'$ and $\tilde{L}$ are compact, A is a Fredholm operator of index 0. The proof is finished if we can show that A is one-to-one.

Assume that $Au=0$ for some $u\in W^1_{0,\partial K}(\Omega_R)$. Then $0=\operatorname{Im}S(u,u)=-\operatorname{Im}\langle L\operatorname{Tr}u,\operatorname{Tr}u\rangle$, and Lemma 1.2(2.) implies $\operatorname{Tr}u=0$. Hence

$$\int_{\Omega_R}\left\{\nabla u\nabla\bar{v}-\kappa^2u\bar{v}\right\}\,\mathrm{d}x=0$$

for all $v\in W^1_{0,\partial K}(\Omega_R)$. Now, it follows from well-known regularity results for weak solutions to elliptic boundary value problems (cf., e.g., [Tay96]) that $u\in C^\infty(\Omega_R)$, $\Delta u+\kappa^2u=0$ in Ω_R, and that u satisfies a classical homogeneous Neumann boundary condition on S_R. Since u vanishing Cauchy data on S_R, the Cauchy-Kovalevskaya Theorem implies that $u=0$ on Ω_R. ∎

1.1.2. Analytic dependence on the domain

To investigate the dependence of the scattered field on the domain, we have to describe domains in some appropriate way. This is done by differentiable functions defined on the boundary ∂K of some fixed reference domain. Differentiabiliy of functions on general sets is defined as follows:

Definition 1.4. A function $g: F\to\mathbb{R}$ defined on a subset $F\subset\mathbb{R}^m$ is called *continuously differentiable* if there exists a continuous function $g': F\to\mathbb{R}^m$ such that for all $x\in F$

$$|g(y)-g(x)-g'(x)\cdot(y-x)|=o(|x-y|)\qquad\text{for } y\to x,\ y\in F. \tag{1.8}$$

A vector valued function $\theta: F\to\mathbb{R}^m$ is called continuously differentiable if all its components are continuously differentiable.

For compact F, $C^1(F)$ is the space of all pairs $\underline{g}=(g,g')$ satisfying (1.8), equipped with the norm

$$\|\underline{g}\|_{C^1(F)}:=\sup_{x\in F}|g(x)|+\sup_{x\in F}|g'(x)|.$$

Note that in general g' is not uniquely determined by g. If, e.g., $F = \partial K$ is smooth, then the tangential component of g' is the surface gradient of g, but the normal component is *not* uniquely determined by g. To avoid this non-uniqueness, an element of $C^1(\partial K)$ is defined as a *pair* (g, g').

For the following analysis, it is important to have C^1 extensions to $\mathbb{R}^m$ of C^1 functions $\underline{g}$ on $F = \partial K$. If F is smooth, such extensions are rather simple to define. For sets F that are merely closed, an extension operator from $C^1(F)$ to $C^1(\mathbb{R}^m)$ was first constructed by Whitney [Whi34] (cf. also [Ste70, VI:§2,§4.7] for a nice exposition). The following theorem gives a variant of this result with the additional requirement that the extension vanish outside an η-neighborhood of F.

Theorem 1.5. *Let $F \subset \mathbb{R}^m$ be closed. Then, for any $\eta > 0$, there exists a bounded linear operator*

$$\mathcal{E}_\eta : C^1(F) \to C^1(\mathbb{R}^m)$$

such that for all $g \in C^1(F)$

$$(\mathcal{E}_\eta g)(x) = g(x), \qquad x \in F, \tag{1.9}$$

$$(\mathcal{E}_\eta g)(x) = 0, \qquad \operatorname{dist}(x, F) \geq \eta. \tag{1.10}$$

Proof. In the references cited above, an extension operator $\mathcal{E}$ is given that satisfies all requirements except (1.10). To additionally meet (1.10), we construct a function $\alpha_\eta \in C^1(\mathbb{R}^m)$ with $\alpha_\eta(x) = 0$ for $\operatorname{dist}(x, F) > \eta$ and $\alpha_\eta(x) = 1$ for $x \in F$, and set

$$(\mathcal{E}_\eta g)(x) := \alpha_\eta(x) \cdot (\mathcal{E} g)(x), \qquad x \in \mathbb{R}^m.$$

An appropriate function α_η can be defined with the regularized distance function $\delta \in C^\infty({}^cF)$ given in [Ste70, Theorem VI,2]. This function satisfies

$$C_1 \operatorname{dist}(x, F) \leq \delta(x) \leq C_2 \operatorname{dist}(x, F) \qquad \text{and}$$
$$|\nabla \delta(x)| \leq C_3$$

for all $x \in {}^cF$ and some constants $C_1, C_2, C_3 > 0$. We choose a function $\chi_\eta \in C^1(\mathbb{R})$ such that $0 \leq \chi_\eta \leq 1$, $\chi_\eta(t) = 1$ for $0 \leq t \leq \frac{C_1\eta}{2}$, and $\chi(t) = 0$ for $t \geq C_1\eta$. Now, we extend δ continuously on F by 0 and set $\alpha_\eta(x) := \chi_\eta(\delta(x))$. Then α_η is continuous on $\mathbb{R}^m$, $\alpha_\eta(x) = 1$ for $\operatorname{dist}(x, F) \leq \frac{C_1\eta}{2C_2}$, $\alpha_\eta(x) = 0$ for $\operatorname{dist}(x, F) \geq \eta$, and

$$|\nabla \alpha_\eta(x)| = |\chi_\eta'(\delta(x)) \nabla \delta(x)| \leq C_3 \|\chi'\|_\infty$$

for $\frac{C_1\eta}{2C_2} \leq \operatorname{dist}(x, F) \leq \eta$. ■

For a vector valued function $\underline{\theta} \in C^1(\partial K, \mathbb{R}^m)$, we define $\mathcal{E}_\eta \underline{\theta}$ componentwise as $(\mathcal{E}_\eta \underline{\theta}_i)_{i=1,\dots,m}$.

Corollary 1.6. *For $\eta > 0$ and $\underline{\theta} \in C^1(\partial K, \mathbb{R}^m)$, $\|\underline{\theta}\| < \|\mathcal{E}_\eta\|^{-1}$, the function $\varphi_{\underline{\theta}} := I + \mathcal{E}_\eta \underline{\theta} : \mathbb{R}^m \to \mathbb{R}^m$ is a diffeomorphism. Consequently, $\varphi_{\underline{\theta}}(K)$ is compact, and $\mathbb{R}^m \backslash \varphi_{\underline{\theta}}(K)$ is connected.*

Proof. For any $a \in \mathbb{R}^m$, Banach's fixed point theorem applied to the equation

$$x = a - \mathcal{E}_\eta \underline{\theta}(x)$$

yields a unique $x \in \mathbb{R}^m$ with $\varphi_{\underline{\theta}}(x) = a$. This shows that $\varphi_{\underline{\theta}}^{-1}$ exists, and by the Inverse Function Theorem it is continuously differentiable. ■

For $\underline{\theta} \in C^1(\partial K, \mathbb{R}^m)$ sufficiently small and $\eta > 0$, let $u[\underline{\theta}]$ be the solution to the weak sound-soft scattering problem for the obstacle $\varphi_{\underline{\theta}}(K)$. Obviously, $u[\underline{\theta}]$ only depends on θ, but not on the derivative $D\theta$, so we write $u[\theta]$ instead of $u[\underline{\theta}]$.

To have a fixed domain of definition we look at the functions

$$\tilde{u}[\underline{\theta}] := u[\theta] \circ \varphi_{\underline{\theta}} \tag{1.11}$$

defined on Ω_R, with $\varphi_{\underline{\theta}}(x) := x + (\mathcal{E}_\eta \underline{\theta})(x)$. In shape optimization the derivative of $\tilde{u}[\underline{\theta}]$ with respect to $\underline{\theta}$ (the existence of which we are going to establish) is called *material derivative*. By the chain rule and a change of variables $y = \varphi_{\underline{\theta}}(x)$, the variational equation

$$S[\underline{\theta}](\tilde{u}[\underline{\theta}], v) = \int_{S_R} \left\{ \frac{\partial u_\mathrm{i}}{\partial \nu} - L u_\mathrm{i} \right\} \bar{v} \, \mathrm{d}s \tag{1.12}$$

holds for all $v \in W^1_{0,\partial K}(\Omega_R)$ with the transformed sesquilinear form

$$\begin{aligned} S[\underline{\theta}](\tilde{u}, v) := & \int_{\Omega_R} \left\{ \nabla \tilde{u} \, (D\varphi_{\underline{\theta}})^{-1} (D\varphi_{\underline{\theta}})^{-t} \nabla \bar{v} - \kappa^2 \tilde{u} \bar{v} \right\} \det(D\varphi_{\underline{\theta}}) \, \mathrm{d}x \\ & - \int_{S_R} L \tilde{u} \, \bar{v} \, \mathrm{d}s. \end{aligned} \tag{1.13}$$

Here, the superscript t denotes the transposed matrix, and $-t$ the inverse of the transposed matrix. Recall the following definition of real analytic functions (cf., e.g., [Die69, Nac69]):

Definition 1.7. Let X, Y be real Banach spaces. A mapping $F : X \supset D(F) \to Y$ is called analytic at x_0 if there exist k-linear, bounded, symmetric mappings $F^{(k)}[x_0] : X \times \cdots \times X \to Y$ for all $k \in \mathbb{N}_0$ and $\rho > 0$ such that for all $h \in X$, $\|h\| < \rho$

$$F[x_0 + h] = \sum_{k=0}^{\infty} \frac{1}{k!} F^{(k)}[x_0](h, \ldots, h).$$

If F is analytic at x_0, then it is C^∞ in a neighborhood of x_0, and the kth derivative at x_0 is $F^{(k)}[x_0]$. An equivalent definition of analyticity is that there exists a complex differentiable local extension $\tilde{F}$ of F to the complexifications of X and Y. From this equivalence it easily follows that compositions of analytic functions are again analytic.

In the following theorem, $\tilde{u}[\underline{\theta}]$ is naturally an element of the *complex* Hilbert space $W^1_{0,\partial K}(\Omega_R)$ whereas $\underline{\theta}$ is in the *real* Banach space $C^1(\partial K; \mathbb{R}^m)$. Therefore, we must interpret $W^1_{0,\partial K}(\Omega_R)$ as a real Hilbert space by introducing the scalar product $\operatorname{Re} \langle u, v \rangle_{W^1(\Omega_R)}$. We also interpret other complex Banach spaces as real Banach spaces.

After these preliminaries we come to the key step in our analysis:

Proposition 1.8. *The mapping*

$$\underline{\theta} \mapsto \tilde{u}[\underline{\theta}], \qquad C^1(\partial K; \mathbb{R}^m) \to W^1_{0,\partial K}(\Omega_R)$$

is analytic at $\underline{\theta} = 0$.

Proof. Since the determinant is a polynomial in the entries of the matrix, $\underline{\theta} \mapsto \det(D\varphi_{\underline{\theta}}) = \det(I + D\mathcal{E}_\eta \underline{\theta})$, $C^1(\partial K; \mathbb{R}^m) \to C(\Omega_R, \mathbb{R})$ is analytic. By the Neumann series

$$(D\varphi_{\underline{\theta}})^{-1} = (I + D\mathcal{E}_\eta \underline{\theta})^{-1} = \sum_{k=0}^{\infty} (-D\mathcal{E}_\eta \underline{\theta})^k,$$

the mapping $\underline{\theta} \mapsto (D\varphi_{\underline{\theta}})^{-1}$, $C^1(\partial K; \mathbb{R}^m) \to C(\Omega_R; \mathbb{R}^{m \times m})$ is analytic at $\underline{\theta} = 0$. Hence, the mapping $\underline{\theta} \mapsto (D\varphi_{\underline{\theta}})^{-t} (D\varphi_{\underline{\theta}})^{-1} \det(D\varphi_{\underline{\theta}})$ is the composition of analytic functions and a bounded 3-linear mapping, so it is analytic at $\underline{\theta} = 0$, and we can expand it into a Taylor series converging in $C(\Omega_R; \mathbb{R}^{m \times m})$. Because of uniform convergence we may interchange summation and integration in the integrals over Ω_R in the definition (1.13) of $S[\underline{\theta}]$. This establishes analyticity of the mapping

$$\underline{\theta} \mapsto S[\underline{\theta}], \qquad C^1(\partial K; \mathbb{R}^m) \to \operatorname{Ses}(W^1_{0,\partial K}(\Omega_R), W^1_{0,\partial K}(\Omega_R)) \tag{1.14}$$

at $\underline{\theta} = 0$. Here $\operatorname{Ses}(W^1_{0,\partial K}(\Omega_R), W^1_{0,\partial K}(\Omega_R))$ is the space of sesquilinear forms on $W^1_{0,\partial K}(\Omega_R)$ with norm $\|A\| := \sup_{\|u\|, \|v\| = 1} |A(u, v)|$. Composing the mapping (1.14) with the canonical isometric isomorphism

$$I : \operatorname{Ses}(W^1_{0,\partial K}(\Omega_R), W^1_{0,\partial K}(\Omega_R)) \to L(W^1_{0,\partial K}(\Omega_R), W^1_{0,\partial K}(\Omega_R)'),$$

we obtain analyticity of the mapping $\underline{\theta} \mapsto A[\underline{\theta}] = I(S[\theta])$.

Finally, note that the mapping inv : $T \mapsto T^{-1}$, $L(X,Y) \supset D(\text{inv}) \to L(Y,X)$ (X, Y Banach spaces) is analytic on its domain. This follows from the Neumann series expansion

$$(T+A)^{-1} = T^{-1}(I + AT^{-1})^{-1} = T^{-1}\sum_{k=0}^{\infty}(-AT^{-1})^k$$

which holds for $\|A\| < \|T^{-1}\|^{-1}$. Since we have shown that

$$\tilde{u}[\underline{\theta}] = (\text{inv} \circ A[\underline{\theta}])\, F$$

is a composition of analytic maps, the proof is complete. ■

Actually, we are not interested in $\tilde{u}[\underline{\theta}]$, but in $u[\theta]$. Note, however, that we cannot speak of analyticity (or even differentiability) of $\theta \mapsto u[\theta]$ in a straightforward manner as the domain of definition of $u[\theta]$ varies with θ. Therefore, we consider the restriction $u[\theta]|_D$ to an arbitrary $D \subset\subset {}^cK$ (i.e. $D \subset {}^cK$ compact and $\text{dist}(D,K) > 0$) with an arbitrary norm $\|\cdot\|_{C^l(D)}$, $l \in \mathbb{N}$. In other words, we establish analyticity of $\underline{\theta} \mapsto u[\theta]$ with respect to all half norms of the locally convex space $C^\infty({}^cK)$.

Theorem 1.9. *For any $D \subset\subset {}^cK$ and any $l \in \mathbb{N}$, the mapping*

$$\underline{\theta} \mapsto u[\theta]|_D\,, \qquad C^1(\partial K; \mathbb{R}^m) \to C^l(D) \tag{1.15}$$

is analytic at $\underline{\theta} = 0$, and all derivatives of $u[\theta]$ satisfy (0.1) and (0.4). Moreover,

$$\underline{\theta} \mapsto u_\infty[\theta], \qquad C^1(\partial K, \mathbb{R}^m) \to L^2(S^{m-1})$$

is analytic at $\underline{\theta} = 0$.

Proof. Without restriction of generality, we assume that $D = B_r := \{x : |x - x_0| < r\}$ with $x_0 \in {}^cK$ and $r > 0$ such that $\text{dist}(B_r, K) > 0$. (Any $D \subset\subset {}^cK$ can be covered by finitely many such balls!) Choose $\eta \in (0, \frac{1}{2}\text{dist}(B_r, K))$ for the extension operator $\mathcal{E}_\eta$. and R such that $B_{r+\eta} \subset B(0,R)$. Then $u[\theta] = \tilde{u}[\underline{\theta}]$ on $B_{r+\eta}$ as $\varphi_{\underline{\theta}}(x) = x$ for $x \in B_{r+\eta}$. Hence, by the previous theorem, $\underline{\theta} \mapsto u[\theta]|_{B_{r+\eta}}$ is analytic with respect to $\|\cdot\|_{W^1(B_{r+\eta})}$. In Green's representation formula

$$u[\theta](x) = \int_{y\in\partial B_{r+\eta}} \left\{ \frac{\partial u[\theta](y)}{\partial\nu}\Phi(x,y) - u[\theta](y)\frac{\partial\Phi(x,y)}{\partial\nu(y)} \right\} \mathrm{d}s(y), \qquad x \in B_r, \tag{1.16}$$

we may differentiate under the integral sign and apply Schwarz's inequality to obtain

$$\begin{aligned}\|D^\alpha u[\theta]\|_{\infty,B_r} &\le \left\|\frac{\partial u[\theta]}{\partial\nu}\right\|_{W^{-1/2}(\partial B_{r+\eta})}\cdot\sup_{x\in B_r}\left\|D_x^\alpha\Phi(x,\cdot)\right\|_{W^{1/2}(\partial B_{r+\eta})}\\ &\quad+\left\|u[\theta]\right\|_{W^{1/2}(\partial B_{r+\eta})}\cdot\sup_{x\in B_r}\left\|D_x^\alpha\frac{\partial\Phi(x,\cdot)}{\partial\nu}\right\|_{W^{-1/2}(\partial B_{r+\eta})}\\ &\le C(\alpha,\eta,m)\cdot\|u[\theta]\|_{W^1(B_{r+\eta})}\end{aligned}$$

for any multi-index α, with a finite constant $C(\alpha,\eta,m)$. Thus, the linear mapping $u[\theta]\mapsto u[\theta]|_{B_r}$, $W^1(B_{r+\eta})\to C^l(B_r)$, given by (1.16), is bounded. This implies analyticity of the mapping (1.15).

To see that derivatives of $u[\theta]$ satisfy the Helmholtz equation, differentiate (1.16) with respect to $\underline{\theta}$. Finally, the assertions on the radiation condition and the far field patterns follow from the formulae

$$\begin{aligned}u_{\rm s}[\theta](x) &= \int_{S_R}\left\{u_{\rm s}[\theta](y)\frac{\partial\Phi(x,y)}{\partial\nu(y)}-\frac{\partial u_{\rm s}[\theta](y)}{\partial\nu}\Phi(x,y)\right\}\mathrm{d}s(y)\quad\text{and}\\ u_\infty[\theta](\hat{x}) &= C_m\int_{S_R}\left\{u_{\rm s}[\theta](y)\frac{\partial e^{-ik\,\hat{x}\cdot y}}{\partial\nu(y)}-\frac{\partial u_{\rm s}[\theta](y)}{\partial\nu}e^{-ik\,\hat{x}\cdot y}\right\}\mathrm{d}s(y),\end{aligned}$$

where $|x|>R$ and $\hat{x}\in S^{m-1}$ (cf. [CK97]). Recall that $u_{\rm s}[\theta]=u[\theta]-u_{\rm i}$. ∎

1.1.3. Boundary values of the derivatives

In the previous section we have established existence of derivatives of $u[\theta]$ of arbitrary order in ${}^cK$. Now, we show that these derivatives have continuous extensions to *smooth* parts of the boundary ∂K and we find expressions for the boundary values. The last part is of particular practical and theoretical interest as, together with Theorem 1.9, it gives a complete characterization of the derivative for smooth boundaries and can be used for numerical implementations.

Since a symmetric n-linear mapping is completely determined by its diagonal values, it suffices to look at the functions $u^{(n)}[\theta](h,\ldots,h)$ and $\tilde{u}^{(n)}[\underline{\theta}](h,\ldots,h)$ which we simply denote by $u^{(n)}[\theta](h)$ and $\tilde{u}^{(n)}[\underline{\theta}](h)$, rsp. If $\underline{\theta}=0$, we drop the argument [0]. Moreover, we use the notation

$$\nabla^l_{(h^1,\ldots,h^l)}w := \sum_{i_1,\ldots,i_l=1}^m h^1_{i_1}\cdots h^l_{i_l}\frac{\partial^l w}{\partial x_{i_1}\cdots\partial x_{i_l}} \tag{1.17}$$

for $h^1,\ldots,h^l\in\mathbb{R}^m$.

Lemma 1.10. *On ^cK, the formula*

$$\tilde{u}^{(n)}(\underline{h}) = \sum_{j=0}^{n} \binom{n}{j} \nabla^j_{(\mathcal{E}_\eta \underline{h},\ldots,\mathcal{E}_\eta \underline{h})}\, u^{(n-j)}(h) \tag{1.18}$$

holds for $\underline{h} \in C^1(\partial K)$.

Proof. For $x_0 \in {}^cK$ we choose $r > 0$ such that $d := \operatorname{dist}(B(x_0, r), K) > 0$. (As opposed to the proof of Theorem 1.9, we do not assume $\eta < d/2$ as this case is trivial here.) Choose a function $\alpha \in C^\infty(\mathbb{R}^m)$, $0 \le \alpha \le 1$, such that $\alpha = 1$ on $B(x_0, r)$ and $\alpha = 0$ outside of $B(x_0, r + d/2)$. We consider the mappings

$$w\left[\begin{pmatrix} x \\ \underline{\theta} \end{pmatrix}\right] := \alpha(x) u[\underline{\theta}](x) \quad \text{and} \quad \tilde{w}\left[\begin{pmatrix} x \\ \underline{\theta} \end{pmatrix}\right] := w\left[\begin{pmatrix} (I + \mathcal{E}_\eta \underline{\theta})(x) \\ \underline{\theta} \end{pmatrix}\right].$$

Due to Theorem 1.9 and the choice of α, w is C^∞ on a neighborhood of $\mathbb{R}^m \times \{0\} \subset \mathbb{R}^m \times C^1(\partial K)$ if w extended by 0 for $x \notin B(x_0, r + d/2)$. By the chain rule, $\tilde{w}$ is C^∞ as well, and

$$\tilde{w}^{(n)}\left[\begin{pmatrix} x \\ \underline{\theta} \end{pmatrix}\right]\left(\begin{pmatrix} 0 \\ \underline{h} \end{pmatrix}\right) = w^{(n)}\left[\begin{pmatrix} (I + \mathcal{E}_\eta \theta)(x) \\ \underline{\theta} \end{pmatrix}\right]\left(\begin{pmatrix} \mathcal{E}_\eta \underline{h}(x) \\ \underline{h} \end{pmatrix}\right).$$

By the symmetry of the derivatives, it follows that

$$\tilde{w}^{(n)}\left(\begin{pmatrix} 0 \\ \underline{h} \end{pmatrix}\right) = \sum_{j=0}^{n} \binom{n}{j} w^{(n)}\Bigg(\underbrace{\begin{pmatrix} \mathcal{E}_\eta \underline{h}(x) \\ 0 \end{pmatrix}}_{j \text{ times}}, \underbrace{\begin{pmatrix} 0 \\ \underline{h} \end{pmatrix}}_{(n-j) \text{ times}}\Bigg)$$

at $(x, 0)$. If $x \in B(x_0, r)$, this is (1.18). Since x_0 was arbitrary, we have proved the assertion. ∎

The left hand side of (1.18) vanishes on ∂K since $\tilde{u}^{(n)} \in W^1_{0,\partial K}(\Omega_R)$. Formally, this gives the desired formula for $u^{(n)}(h)$ in terms of lower order Fréchet derivatives (cf. (1.19) below). To make this rigorous, we have to establish regularity properties of the Fréchet derivatives. This is done by the following standard regularity result:

Lemma 1.11. *Assume that Ω_R is C^{1+l}-smooth ($l \in \mathbb{N}_0$) in $x_0 \in \partial K$, i.e. there exists a neighborhood G of x_0 in $\overline{\Omega_R}$ with the following properties: There exist orthogonal coordinates $y_1, \ldots, y_m$ related to $x_1, \ldots x_m$ by an affinely linear transformation and a function $\psi \in C^l(W_\epsilon)$, $W_\epsilon := \{y' \in \mathbb{R}^{m-1} : |y'| < \epsilon\}$, $\epsilon > 0$ such that*

$$G \cap \partial\Omega_R = \psi(W_\epsilon) \text{ and } G = \{(y', y_m) \in W_\epsilon \times \mathbb{R} : \psi(y') \le y_m < \psi(y') + \epsilon\}.$$

Let w be a solution to the Helmholtz equation in $G \backslash \partial\Omega_R$, and assume that $w \in W^1(U)$ with $\operatorname{Tr} w \in W^{l+1/2}(U \cap \partial\Omega_R)$ for any compact $U \subset G$. Then $w \in W^{1+l}(U)$ for any compact $U \subset G$.

Proof. This is a special case of regularity theorems for more general elliptic partial differential equations that can be found, e.g. in [GT77, RR92]. For a discussion of other equivalent definitions of boundary regularity, we refer to [Wlo82]. ■

Theorem 1.12. *Assume that Ω_R is C^{1+l}-smooth in $x_0 \in \partial K$ ($l \in \mathbb{N}_0$) and that $x_0 \in G \subset \overline{\Omega_R}$ as in Lemma 1.11. Then, for $h \in C^1(\partial K) \cap C^{1+l}(G \cap \partial K)$, the derivatives $u^{(n)}(h)$, $n \in \{0, \ldots, l\}$ belong to $W^{1+l-n}(U)$ for any compact subset $U \subset G$, and the formula*

$$\operatorname{Tr} u^{(n)}(h) = -\sum_{j=1}^{n} \binom{n}{j} \operatorname{Tr} \nabla^j_{(h,\ldots,h)} u^{(n-j)}(h) \tag{1.19}$$

holds for the trace operator on $U \cap \partial K$.

Proof. We prove the assertion by induction on n. For $n = 0$, $\operatorname{Tr} u = 0$ holds by definition, and Lemma 1.11 implies $u \in W^{1+l}(U)$. Assume the assertion is true for $n - 1$. Eq. (1.18) yields

$$u^{(n)}(h) = \tilde{u}^{(n)}(\underline{h}) - \sum_{j=1}^{n} \binom{n}{j} \nabla^j_{(\mathcal{E}_\eta \underline{h},\ldots,\mathcal{E}_\eta \underline{h})} u^{(n-j)}(h) \quad \text{on } \Omega_R. \tag{1.20}$$

The induction hypothesis implies the sum on the right hand side has a trace in $W^{l-n+1/2}(U \cap \partial K)$ for any compact $U \subset G$. Moreover, $\operatorname{Tr} \tilde{u}^{(n)}(\underline{h}) = 0$ as $\tilde{u}^{(n)}(\underline{h}) \in W^1_{0,\partial K}$, and $(\Delta + \kappa^2)u^{(h)}(h) = 0$ by Theorem 1.9. Therefore, Lemma 1.11 implies $u^{(n)}(h) \in W^{l-n+1}(U)$, and (1.19) holds for n. ■

Remark 1.13. A numerical evaluation of Fréchet derivatives for irregular domains, e.g. domains with corners or open arcs, still requires some additional work since the boundary values of the derivatives have singularities at points where ∂K is not smooth. Therefore, numerical code to calculate u cannot be used in a straightforward way to compute $u'(h)$. Here the regularity of $\tilde{u}'(h)$, i.e. $\tilde{u}'(h) \in W^1_{0,\partial K}(\Omega_R)$ can be useful (cf. Kress [Kre95a, Kre95b]). We mention that using regularity results in [GT77, Chapters 6 and 8], it can be shown that the total derivatives $\tilde{u}^{(n)}(h)$ are continuous or even locally Hölder continuous up to the boundary under very general assumptions on K, and that the boundary values in (1.19) are actually attained in the classical sense. However, we do not go into details since we do not need these results here.

1.2. Neumann boundary conditions

1.2.1. The sound-hard scattering problem

Let $K \subset \mathbb{R}^m$, be compact, ${}^cK := \mathbb{R}^m \backslash K$ connected, and assume that ${}^cK$ has the cone property which is defined as follows:

Definition 1.14. Let $x \in \mathbb{R}^m$ and B a ball with $x \notin B$. Then

$$C_x^B := \{x + \lambda(y - x) : \lambda \in (0,1), y \in B\}$$

is called a *finite cone with vertex x*.

An open domain $\Omega \subset \mathbb{R}^m$ has the *cone property* if there exists a finite cone C such that each point $x \in \Omega$ is the vertex of a finite cone C_x contained in Ω and congruent to C.

Obviously, for R sufficiently large, ${}^cK$ has the cone property if and only if $\Omega_R := \{x \in {}^cK : |x| < R\}$ has the cone property. If this is true, the embedding $W^1(\Omega_R) \hookrightarrow L^2(\Omega_R)$ is compact (cf. [Ada75, Theorem 6.2]), and this is what we actually need. Note that Ω_R has the cone property if, e.g., K is a polyhedron or an open arc.

Problem 1.2. Let $u_\mathrm{i} \in C^2(\mathbb{R}^m)$ be an incident field solving the Helmholtz equation $\Delta u_\mathrm{i} + \kappa^2 u_\mathrm{i} = 0$ in $\mathbb{R}^m$. A function $u_\mathrm{s} \in C^2({}^cK)$ is called a *solution to the sound-hard scattering problem* for u_i if it satisfies the conditions (0.1) and (0.4), and if $u := u_\mathrm{i} + u_\mathrm{s}$ satisfies the boundary condition $\frac{\partial u}{\partial \nu}\big|_{\partial K} = 0$ in the sense that $u \in W^1(\Omega_R)$ and

$$S(u, v) = F(v) \tag{1.21}$$

for all $v \in W^1(\Omega_R)$ with F given by (1.2) and

$$S(u, v) := \int_{\Omega_R} \{\nabla u \cdot \nabla \bar{v} - \kappa^2 u \bar{v}\}\, \mathrm{d}x - \int_{S_R} Lu\, \bar{v}\, \mathrm{d}s.$$

Of course, as in Lemma 1.1, if $u \in W^1(\Omega_R)$ is a solution to (1.21) then $u_\mathrm{s} = u - u_\mathrm{i}$ can be extended such that (0.1) and (0.4) are satisfied. Therefore, we may consider a solution to (1.21) as a solution to the sound-hard scattering problem. If the boundary is smooth, the condition $\frac{\partial u}{\partial \nu}\big|_{\partial K} = 0$ is satisfied in the sense of the trace operator.

The proof of the following existence and uniqueness theorem is analogous to the proof of Theorem 1.3, and needs the compactness of the embedding $W^1(\Omega_R) \hookrightarrow L^2(\Omega_R)$ (cf. [Het95]).

Theorem 1.15. *The operator $A : W^1(\Omega_R) \to W^1(\Omega_R)'$, defined implicitely by*

$$S(u,v) = \langle Au, v\rangle_{L^2(\Omega_R)} \qquad \text{for all } u,v \in W^1(\Omega_R), \tag{1.22}$$

is bounded and boundedly invertible. Consequently, the sound-hard scattering problem has a unique solution $u = A^{-1}F$ for all incident waves u_{i}.

1.2.2. Analytic dependence on the domain

We have the same setting as in §1.1.2.. To assure that the sound-hard scattering problem has a solution for small variations of the domain K, we additionally need the following lemma:

Lemma 1.16. *Assume that $\Omega \subset \mathbb{R}^m$ has the cone property. Then $\varphi_{\underline{\theta}}(\Omega)$ has the cone property for small $\underline{\theta} \in C^1(\mathbb{R}^m, \mathbb{R}^m)$.*

Proof. Assume that Ω has the cone property with reference cone $C_0^{B(m,r)}$, i.e. for any $x \in \Omega$ there exists a cone $C_x^{B(m_x,r_x)} \subset \Omega$ congruent to $C_0^{B(m,r)}$. We show that $\theta(x) + C_x^{B(m_x,r_x/2)} \subset \varphi_{\underline{\theta}}(C_x^{B(m_x,r_x)}) \subset \varphi_{\underline{\theta}}(\Omega)$ for small $\underline{\theta}$, which implies that $\varphi_{\underline{\theta}}(\Omega)$ has the cone property with reference cone $C_0^{B(m,r/2)}$. Without restriction of generality $x = 0$. Note that $C_0^{B(m,r)} = \bigcup_{\lambda\in(0,1)} B(\lambda m, \lambda r)$. Hence, we have to show that $\theta(0) + B(\lambda m, \lambda\frac{r}{2}) \subset \varphi_{\underline{\theta}}(B(\lambda m, \lambda r))$, or, equivalently,

$$\psi(\theta(0) + B(\lambda m, \lambda\frac{r}{2})) \subset B(\lambda m, \lambda r) \tag{1.23}$$

with $\psi := \varphi_{\underline{\theta}}^{-1}$. For $y \in B(\lambda m, \lambda\frac{r}{2})$, we have

$$\begin{aligned} |\psi\left(\theta(0) + y\right) - \lambda m| &= \left|\psi(\varphi_{\underline{\theta}}(0)) + \int_0^1 D\psi(\varphi_{\underline{\theta}}(0) + \tau y) y \,\mathrm{d}\tau - \lambda m\right| \\ &\leq |y - \lambda m| + \|D\psi - I\| |y| \\ &\leq \frac{r}{2} + \|D\psi - I\|(m + \frac{r}{2}). \end{aligned}$$

We have $D\psi \circ \varphi_{\underline{\theta}} = (D\varphi_{\underline{\theta}})^{-1} = \sum_{j=0}^{\infty}(-D\theta)^j$ by the Inverse Function Theorem and the Neumann series, so $\|D\psi - I\| \leq \frac{1}{1-\|D\theta\|} - 1 = \frac{\|D\theta\|}{1-\|D\theta\|}$. Thus, (1.23) holds for $\|D\theta\| \leq \frac{r}{2m+r}$, which proves the assertion. ■

Completely analogous to Proposition 1.8 and Theorem 1.9, we have the following result:

Theorem 1.17. *For any $D \subset\subset {}^cK$ and any $l \in \mathbb{N}$, the mappings*

$$\begin{aligned} &\underline{\theta} \mapsto \tilde{u}[\underline{\theta}], && C^1(\partial K, \mathbb{R}^m) \to W^1(\Omega_R) \\ &\underline{\theta} \mapsto u[\theta]|_D, && C^1(\partial K, \mathbb{R}^m) \to C^l(D) \\ &\underline{\theta} \mapsto u_\infty[\theta], && C^1(\partial K, \mathbb{R}^m) \to L^2(S^{m-1}) \end{aligned}$$

are analytic at $\underline{\theta} = 0$. All derivatives of $u[\theta]$ are radiating solutions to the Helmholtz equation in ${}^cK$.

1.2.3. Boundary values of the derivatives

We need the following regularity result:

Lemma 1.18. *Let Ω_R be $C^{1+l,1}$-smooth in a $x_0 \in \partial K$ with G as in Lemma 1.11. Moreover, let $f \in W^{l-1}(U)$ and $g \in W^{l-1/2}(\partial\Omega_R \cap U)$ for any compact $U \subset G$, and assume that $w \in W^1(\Omega)$ is a solution to the variational equation*

$$\int_{\Omega_R} \left\{ \nabla u \nabla \bar{v} - \kappa^2 u \bar{v} \right\} \mathrm{d}x = \int_{\Omega_R} f \bar{v} \, \mathrm{d}x + \int_{\partial\Omega_R} g \bar{v} \, \mathrm{d}s$$

for all $v \in W^1(\Omega)$ with $\operatorname{supp} v \subset G$. Then $u \in W^{l+1}(U)$ for all compact $U \subset G$.

Proof. This follows from more general regularity theorems in [Neč67] or [Wlo82]. ∎

The Fréchet derivatives $u^{(n)}(h)$ have the following Neumann boundary values on smooth parts of ∂K:

Theorem 1.19. *Let $\partial\Omega_R$ be $C^{1+l,1}$-smooth in $x_0 \in \partial K$ with G as in Lemma 1.11, and let $h \in C^1(\partial K) \cap C^l(G \cap \partial K)$. Then the derivatives have the regularity*

$$\tilde{u}^{(n)}(h) \in W^{1+l}(U) \qquad n \in \{0, 1, \dots\}, \tag{1.24}$$

$$u^{(n)}(h) \in W^{l+1-n}(U) \qquad n \in \{0, \dots, l\} \tag{1.25}$$

for any compact subset $U \subset G$, and the functions $u^{(n)}(h)$ and satisfy the boundary condition

$$\begin{aligned} \operatorname{Tr} \nabla_\nu u^{(n)}(h) = &- \sum_{j=1}^{n} \binom{n}{j} \operatorname{Tr} \nabla^{j+1}_{(h,\dots,h,\nu)} u^{(n-j)}(h) - \\ &- \sum_{j=1}^{n} \binom{n}{j} \operatorname{Tr} \nabla_{\tilde{\nu}^{(j)}(\underline{h})} \tilde{u}^{(n-j)}(\underline{h}) \end{aligned} \tag{1.26}$$

with $\tilde{\nu}[\underline{\theta}] := (D\varphi_{\underline{\theta}}^t D\varphi_{\underline{\theta}})^{-1}\det(D\varphi_{\underline{\theta}})\nu[0]$. *Here* Tr *is the trace operator on* $U \cap \partial K$, *and the notation* $\nabla \ldots$ *is defined in (1.17).*

Proof. Recall that $S[\underline{\theta}]$ is given by

$$S[\underline{\theta}](w,v) = \int_{\Omega_R} \{\nabla w M[\underline{\theta}]\nabla\bar{v} + wN[\underline{\theta}]\bar{v}\}\,\mathrm{d}x - \int_{S_R} Lw\,\bar{v}\,\mathrm{d}s$$

with the matrix-valued function $M[\underline{\theta}] = (D\varphi_{\underline{\theta}}^t D\varphi_{\underline{\theta}})^{-1}\det(D\varphi_{\underline{\theta}})$ and the scalar function $N[\underline{\theta}] := -\kappa^2\det(D\varphi_{\underline{\theta}})$ which both depend analytically on $\underline{\theta}$. Differentiating (1.12) n times yields

$$\int_{\Omega_R}\left\{\nabla\tilde{u}^{(n)}\nabla\bar{v} - \kappa^2\tilde{u}^{(n)}\bar{v}\right\}\mathrm{d}x = \\ -\sum_{j=1}^{n}\binom{n}{j}\int_{\Omega_R}\left\{\nabla\tilde{u}^{(n-j)}M^{(j)}\nabla\bar{v} + \tilde{u}^{(n-j)}N^{(j)}\bar{v}\right\}\mathrm{d}x$$

for $v \in W^1(\Omega_R)$ with $\operatorname{supp} v \subset G$. We have assumed that R is sufficiently large such that $G \cap S_R = \emptyset$ and dropped the argument $(\underline{h})$ of the Fréchet derivatives. We proceed by induction on n to prove (1.24):

For $n = 0$, the right hand side of the last equation is 0, so the assertion follows from Lemma 1.18. Assume that (1.24) holds for all Fréchet derivatives up to order $n-1$. The extension operator can be chosen such that $\mathcal{E}_\eta\underline{h} \in C^{l+1}(G)$ (cf. [Ste70]). Since all entries of all derivatives of $M[\underline{\theta}]$ at $\underline{\theta} = 0$ are polynomials in entries of $D\mathcal{E}_\eta\underline{h}$, we have $M^{(k)} \in C^l(G, \mathbb{R}^{m\times m})$ for all $k \in \mathbb{N}$, and analogously, $N^{(k)} \in C^l(G, \mathbb{R})$. Therefore, an application of Gauß' divergence theorem in G and the relation $\left\langle (M^{(j)})^t\nabla\tilde{u}^{(n-j)}, \nu\right\rangle = \nabla_{\tilde{\nu}^{(j)}}\tilde{u}^{(n-j)}$ yield

$$\int_{\Omega_R}\left\{\nabla\tilde{u}^{(n)}\nabla\bar{v} - \kappa^2\tilde{u}^{(n)}\bar{v}\right\}\mathrm{d}x = -\sum_{j=1}^{n}\binom{n}{j}\int_{G\cap\partial K}\operatorname{Tr}\left\{\nabla_{\tilde{\nu}^{(j)}}\tilde{u}^{(n-j)}\right\}\operatorname{Tr}\bar{v}\,\mathrm{d}s \\ -\sum_{j=1}^{n}\binom{n}{j}\int_{\Omega_R}\left\{\nabla(M^{(j)})^t\nabla\tilde{u}^{(n-j)} + \tilde{u}^{(n-j)}N^{(j)}\right\}\bar{v}\,\mathrm{d}x. \tag{1.27}$$

Now (1.24) for n follows from Lemma 1.18, the induction hypothesis, and the trace theorem.

(1.25) now follows from (1.18) and (1.24) by induction on n. (1.24) and (1.27) imply

$$\operatorname{Tr}\nabla_\nu\,\tilde{u}^{(n)} = -\sum_{j=1}^{n}\binom{n}{j}\operatorname{Tr}\nabla_{\tilde{\nu}^{(j)}}\tilde{u}^{(n-j)}.$$

Plugging (1.18) into this equation gives (1.26). ■

1.3. Other forms of the boundary values of the derivatives

In this section we derive alternative forms of the boundary values of the Fréchet derivatives derived in Theorems 1.12 and 1.19. These alternative expressions are better suited for numerical implementations although in most cases they look more complicated. For Dirichlet boundary conditions and $m \in \{2,3\}$ we have

$$\operatorname{Tr} u'(h) = -\operatorname{Tr} \nabla u \cdot h = -\frac{\partial u}{\partial \nu} \langle h, \nu \rangle \tag{1.28}$$

since the tangential part of ∇u vanishes due to the boundary condition. If Problem 1.1 is solved by an integral equation method as discussed in Chapter 2, then $\frac{\partial u}{\partial \nu}$ arises as solution of an integral equation. Therefore, the right hand side of (1.28) can easily be evaluated.

Corresponding transformations for higher derivatives and other boundary conditions involve some elementary differential geometry that is provided below. The aim is to express the right hand sides of (1.19) and (1.26) in terms of the Cauchy data of the total field, i.e. u and $\frac{\partial u}{\partial \nu}$ using essentially only the following operations:

- tangential derivatives
- Dirichlet-to-Neumann or Neumann-to-Dirichlet maps

Using boundary integral equations Dirichlet-to-Neumann and Neumann-to-Dirichlet maps are straightforward to implement. Computation of tangential derivatives requires some care since numerical differentiation is unstable. In Chapter 2 we describe a stable and efficient algorithm to calculate tangential derivatives for $m = 2$.

Tools from differential geometry: Let $\Gamma \subset \mathbb{R}^3$ be a C^2-smooth part of a surface, $\nu : \Gamma \to \mathbb{R}^3$ a unit length normal vector, and $x : \mathbb{R}^2 \supset W \to \Gamma$ a C^2-parametrization such that the vectors $x_{,i}(w) := \frac{\partial x}{\partial w_i}$ are linearly independent and that

$$\nu = \frac{x_{,1} \times x_{,2}}{|x_{,1} \times x_{,2}|}.$$

For $x_0 \in \Gamma$ let $\mathrm{P}_{x_0} X := X - \nu(x_0) \langle X, \nu(x_0) \rangle$, $X \in T_{x_0}\mathbb{R}^3 \sim \mathbb{R}^3$ denote the orthogonal projection onto the tangent space $T_{x_0}\Gamma$ of Γ at x_0.

With the convention to sum over equal subscripts and superscripts, the inner product of tangent vectors $X = X^i x_{,i}$ and $Y = Y^i x_{,i}$ induced by the inner product of $\mathbb{R}^3$ is given by

$$\langle X, Y\rangle = X^i Y^j g_{ij} \quad \text{with} \quad g_{ij} := \langle x_{,i}\,, x_{,j}\rangle\,.$$

We set $g := \det(g_{ij})$ and denote by (g^{ij}) the inverse matrix of (g_{ij}).

If $c : [0,1] \to \Gamma$ is a smooth curve on Γ with $c(0) = x_0$, we define the derivative of ν in the direction $c'(0)$ by $\nabla_{c'(0)}\,\nu(x_0) := (\nu \circ c)'(0)$. Since

$$0 = \frac{d}{dt}|(\nu \circ c)(t)|^2_{|t=0} = 2\,\langle \nu(x_0), (\nu \circ c)'(0)\rangle\,,$$

the *Weingarten map* $L_{x_0} : T_{x_0}\Gamma \to T_{x_0}\Gamma$ is well defined by

$$L_{x_0} X := \nabla_X\,\nu. \tag{1.29}$$

It is easily seen that L_{x_0} is symmetric, i.e. $\langle L_{x_0}X, Y\rangle = \langle X, L_{x_0}Y\rangle$ for all $X, Y \in T_{x_0}\Gamma$. The eigenvalues κ_1, κ_2 of L_{x_0} are called *principal curvatures* of Γ at x_0. The *mean curvature* $H(x_0)$ and the *Gaussian curvature* $G(x_0)$ of Γ at x_0 are defined by [1]

$$H(x_0) := \frac{1}{2}(\kappa_1 + \kappa_2) \quad \text{and} \quad G(x_0) := \kappa_1\kappa_2,$$

i.e. $H(x_0) = \frac{1}{2}\operatorname{Tr} L_{x_0}$ and $G(x_0) = \det L_{x_0}$.

We frequently work with the coordinates

$$\tilde{x}(w', w_3) := x(w') + w_3\nu(x(w')) \qquad w' = (w_1, w_2) \in W,\ |w_3| < \epsilon$$

in the tubular neighborhood $U_\epsilon(\Gamma) := \tilde{x}(W \times (-\epsilon, \epsilon))$ of Γ.

Lemma 1.20. *$\tilde{x}$ is locally injective for sufficiently small $|w_3|$, and the metric tensor $\tilde{g} := \det(D\tilde{x}^* D\tilde{x})$ is given by*

$$\tilde{g}(w) = g(w')\big(1 + 2w_3H(w') + w_3^2G(w')\big)^2. \tag{1.30}$$

Proof. It follows from definition (1.29) that $\frac{\partial \tilde{x}}{\partial w'}(w) = (I + w_3 L_{x(w')})Dx(w')$. With this relation, it is easily seen that $V := \operatorname{span}\{\nu(x(w'))\} = \operatorname{ran}(\frac{\partial \tilde{x}}{\partial w_3})$ and

[1] There are different sign conventions for the Weingarten map. Therefore, some of the formulae below appear with a different sign in front of H in the literature ([Mar68, SW]). We have defined L such that a sphere with outward pointing normal vector has positive mean curvature H.

the tangent space $V^\perp = \operatorname{ran}(\frac{\partial \tilde{x}}{\partial w'})$ are invariant subspaces of $D\tilde{x}(w)D\tilde{x}^*(w)$ and that

$$\det(D\tilde{x}D\tilde{x}^*\big|_{V^\perp}) = \det(I + w_3L)^2 \det(Dx^*Dx).$$

Since $D\tilde{x}D\tilde{x}^*|_V = |\nu(x(w'))|^2 = 1$ and since the eigenvalues of $I + w_3L$ are $1 + w_3\kappa_i$, $i = 1, 2$, this gives (1.30). The inverse function theorem implies that $\tilde{x}$ is injective in a neighborhood of w if $\tilde{g}(w) \neq 0$ which holds for small $|w_3|$. ■

We sometimes silently extend scalar or vector valued functions X defined on Γ to $U_\epsilon(\Gamma)$ by

$$X(\tilde{x}(w', w_3)) := X(x(w')). \tag{1.31}$$

We now derive some relations between differential operators defined on Γ and the corresponding operators in $U_\epsilon(\Gamma)$. In the following, Latin indices run over $1, \ldots, m-1$ and Greek indices over $1, \ldots, m$. We use the notations $\partial_\mu := \frac{\partial}{\partial w_\mu}$.

The surface gradient $(\operatorname{Grad}\phi)(x_0) \in T_{x_0}\Gamma$ of a scalar function of Γ is defined by its action on tangential vectors $c'(0)$ where $c : [0,1] \to \Gamma$ is a smooth curve with $c(0) = x_0$:

$$\langle \operatorname{Grad}\phi(x), c'(0)\rangle := (\phi \circ c)'(0)$$

In local coordinates $\operatorname{Grad}\phi$ can be computed by the formula

$$\operatorname{Grad}\phi = g^{jk}\partial_j x_{,k},$$

and if $\phi \in C^1(U_\epsilon(\Gamma))$ then

$$\operatorname{Grad}\phi = \mathrm{P}\operatorname{grad}\phi \qquad \text{on } \Gamma.$$

The surface divergence of a tangential vector field $X = X^i x_{,i}$ is defined by

$$\operatorname{Div}(X) := g^{-1/2}\partial_i\big(g^{1/2}X^i\big).$$

It can be shown that this definition is independent of the choice of coordinates. For $Y = Y^\mu \tilde{x}_{,\mu} \in C^1(U_\epsilon(\Gamma), \mathbb{R}^3)$, it follows from (1.30) that

$$\begin{aligned} \operatorname{div} Y\big|_\Gamma &= \tilde{g}^{-1/2}\partial_\mu\big(\tilde{g}^{1/2}Y^\mu\big)\big|_\Gamma \\ &= g^{-1/2}\partial_i\big(g^{1/2}Y^i\big) + \partial_3 Y^3 - 2HY^3\big|_\Gamma \\ &= \operatorname{Div}\mathrm{P}Y + \partial_3\langle Y, \nu\rangle + 2H\langle Y, \nu\rangle\big|_\Gamma. \end{aligned} \tag{1.32}$$

The Laplace-Beltrami operator on Γ is defined by $\Delta_\Gamma \phi := \operatorname{Div} \operatorname{Grad} \phi$. From our previous calculations it follows that Δ_Γ is related to the Laplace operator $\Delta = \operatorname{div} \operatorname{grad}$ in $U_\epsilon(\Gamma)$ by

$$\begin{aligned} \Delta\phi\big|_\Gamma &= \operatorname{Div} \mathrm{P} \operatorname{grad} \phi + \partial_3 \langle \operatorname{grad} \phi, \nu \rangle + 2H \langle \operatorname{grad} \phi, \nu \rangle \big|_\Gamma \\ &= \Delta_\Gamma \phi + \partial_3^2 \phi + 2H \partial_3 \phi\big|_\Gamma . \end{aligned} \tag{1.33}$$

Finally, we note that the identity

$$\nabla^2_{(f,g)} u = \nabla_f \nabla_g u - \nabla_{\nabla_g f} u. \tag{1.34}$$

holds for $f \in C^1({}^cK, \mathbb{R}^m)$, $g \in C({}^cK, \mathbb{R}^m)$ with $\nabla^2_{(f,g)} u$ defined by (1.17).

With these tools we can prove the following results:

Proposition 1.21. *Under the assumptions of Theorem 1.12 with $m = 3$ and $n = 2$ the following formula holds:*

$$\operatorname{Tr} u''(h) = -2h^\nu \frac{\partial u'(h)}{\partial \nu} + \left(2\nabla_{\mathrm{P}h} h^\nu + 2H(h^\nu)^2 - \langle L\mathrm{P}h, \mathrm{P}h\rangle\right) \frac{\partial u}{\partial \nu} \tag{1.35}$$

Proof. The formula of Theorem 1.12 is

$$u''(h) = -2\nabla_h u'(h) - \nabla^2_{(h,h)} u. \tag{1.36}$$

Here and in the rest of this proof, we omit the trace operator. Due to the decomposition $h = h^\nu \nu + \mathrm{P}h$ and (1.28), the first term satisfies

$$-2\nabla_h u'(h) = -2h^\nu \frac{\partial u'(h)}{\partial \nu} + 2\nabla_{\mathrm{P}h} \left(h^\nu \frac{\partial u}{\partial \nu}\right),$$

and the second term can be decomposed into

$$-\nabla^2_{(h,h)} u = -\nabla^2_{(h^\nu \nu, h^\nu \nu)} u - 2\nabla^2_{(h^\nu \nu, \mathrm{P}h)} u - \nabla^2_{(\mathrm{P}h, \mathrm{P}h)} u. \tag{1.37}$$

Since $\partial_3 \nu = 0$ (cf. (1.31)), we have $\nabla^2_{(\nu,\nu)} u = \partial_3^2 u$. It follows from (1.33), the boundary condition, and the Helmholtz equation that

$$\nabla^2_{(h^\nu \nu, h^\nu \nu)} u = -H(h^\nu)^2 \frac{\partial u}{\partial \nu}.$$

To find an expression for the second term in (1.37), we first note that

$$\begin{aligned} \nabla_{\nabla_{\mathrm{P}h}(h^\nu \nu)} u &= \langle \nabla_{\mathrm{P}h} (h^\nu \nu), \nabla u \rangle = \langle \nabla_{\mathrm{P}h} (h^\nu \nu), \nu \rangle \frac{\partial u}{\partial \nu} \\ &= \left(\nabla_{\mathrm{P}h} h^\nu + h^\nu \langle \nabla_{\mathrm{P}h} \nu, \nu \rangle\right) \frac{\partial u}{\partial \nu} = \left(\nabla_{\mathrm{P}h} h^\nu\right) \frac{\partial u}{\partial \nu} \end{aligned}$$

as $0 = \nabla_{\mathrm{P}h} \langle \nu, \nu \rangle = 2 \langle \nabla_{\mathrm{P}h} \nu, \nu \rangle$. Together with (1.34) this yields

$$\nabla^2_{(h^\nu \nu, \mathrm{P}h)} u = \nabla_{\mathrm{P}h} \left(h^\nu \frac{\partial u}{\partial \nu} \right) - (\nabla_{\mathrm{P}h} h^\nu) \frac{\partial u}{\partial \nu}.$$

For $x_0 \in \Gamma$ let $c : [0,1] \to \Gamma$ be a C^2-curve with $c(0) = x_0$ and $c'(0) = \mathrm{P}h(x_0)$. Then

$$\begin{aligned} 0 &= (u \circ c)''(0) = \frac{d}{dt} \langle \nabla u(c(t)), c'(t) \rangle \big|_{t=0} \\ &= \nabla^2_{(c'(0), c'(0))} u(x_0) + \frac{\partial u}{\partial \nu}(x_0) \langle \nu(c(0)), c''(0) \rangle . \end{aligned}$$

Differentiating the equation $0 = \langle \nu(c(t)), c'(t) \rangle$ yields

$$\langle \nu(c(0)), c''(0) \rangle = - \langle (\nu \circ c)'(0), c'(0) \rangle = - \langle Lc'(0), c'(0) \rangle .$$

Therefore,

$$\nabla^2_{(\mathrm{P}h, \mathrm{P}h)} u = \langle L\mathrm{P}h, \mathrm{P}h \rangle \frac{\partial u}{\partial \nu}.$$

Putting everything together gives the assertion. ■

Remark 1.22. We consider the case $m = 2$. A smooth planar curve $c : [0,1] \to \mathbb{R}^2$ has only one curvature H. If c is parametrized by the arc-length, i.e. $|c'| = 1$, then $c'' = -H\nu$. The Weingarten map L simply becomes a multiplication by H. The formulae (1.30), (1.32), and (1.33) have to be replaced by

$$\begin{aligned} \tilde{g}(w_1, w_2) &= g(w_1)\big(1 + w_2 H(w_1)\big) && (1.38) \\ \operatorname{div} Y\big|_\Gamma &= \operatorname{Div} \mathrm{P}Y + \partial_2 \langle Y, \nu \rangle + H \langle Y, \nu \rangle \big|_\Gamma && (1.39) \\ \Delta\phi\big|_\Gamma &= \Delta_\Gamma \phi + \partial_2^2 \phi + H \partial_2 \phi\big|_\Gamma . && (1.40) \end{aligned}$$

Actually, both Div and Grad essentially reduce to the arc-length derivative $\frac{df}{ds}(c(t)) := (f \circ c)'(t)$. If $\tau := c'(t)$ then

$$\operatorname{Div}(f\tau) = \frac{df}{ds} \qquad \text{and} \qquad \operatorname{Grad} f = \frac{df}{ds}\tau.$$

Therefore, (1.35) becomes

$$u''(h) = -2h^\nu \frac{\partial u'(h)}{\partial \nu} + \left(2h^\tau \frac{dh^\nu}{ds} + H(h^\nu)^2 - H(h^\tau)^2 \right) \frac{\partial u}{\partial \nu} \qquad (1.41)$$

with $h^\tau := \langle h, \tau \rangle$.

Remark 1.23. The non-diagonal values of the second derivative can be recovered from the diagonal values by

$$2u''(h_1, h_2) = u''(h_1 + h_2) - u''(h_1) - u''(h_2).$$

In case of (1.41) this gives the formula

$$\begin{aligned} u''(h_1, h_2) = &- h_1^\nu \frac{\partial u'(h_2)}{\partial \nu} - h_2^\nu \frac{\partial u'(h_1)}{\partial \nu} \\ &+ \left(h_1^\tau \frac{dh_2^\nu}{ds} + h_2^\tau \frac{dh_1^\nu}{ds} + H h_1^\nu h_2^\nu - H h_1^\tau h_2^\tau \right) \frac{\partial u}{\partial \nu} \end{aligned} \tag{1.42}$$

which corresponds to a result by Hettlich and Rundell [HR, Theorem 6.1].

Proposition 1.24. *Under the assumptions of Theorem 1.19 with $m = 3$ and $n = 1$ the following formula holds:*

$$\frac{\partial u'(h)}{\partial \nu} = \langle \operatorname{Grad} h^\nu, \operatorname{Grad} u \rangle + h^\nu (\Delta_\Gamma + \kappa^2) u \tag{1.43}$$

Proof. The formula from Theorem 1.19 is

$$\begin{aligned} \frac{\partial u'(h)}{\partial \nu} &= -\nabla^2_{(h,\nu)}\, u - \langle \tilde{\nu}'(h), \nabla u \rangle \\ &= -h^\nu \nabla^2_{(\nu,\nu)}\, u - \nabla^2_{(\mathrm{P}h,\nu)}\, u - \langle \tilde{\nu}'(h), \nabla u \rangle\,. \end{aligned}$$

(1.33), (0.1) and (0.3) yield

$$-\nabla^2_{(\nu,\nu)}\, u = \Delta_\Gamma u + \kappa^2 u.$$

From (1.34), $\frac{\partial u}{\partial \nu} = 0$, and the definition (1.29) we obtain

$$-\nabla^2_{(\mathrm{P}h,\nu)}\, u = -\nabla_{\mathrm{P}h} \frac{\partial u}{\partial \nu} + \nabla_{\nabla_{\mathrm{P}h}\, \nu}\, u = \nabla_{L(\mathrm{P}h)}\, u.$$

By the differentiation formula $(A^{-1})'[0](h) = -A^{-1}[0]\, A'[0](h) A^{-1}[0]$ we have

$$\tilde{\nu}'[0](\underline{h}) \;=\; -(D\underline{h})^t \nu - (D\underline{h})\nu + \big(\det D\varphi_{\underline{0}}\big)'[0](\underline{h})\nu.$$

If h is extended according to (1.31) near Γ, then $(Dh)\nu = \partial_3 h = 0$. Therefore,

$$\begin{aligned} -\langle \tilde{\nu}'[0](\underline{h}), \nabla u \rangle &= \langle \nu, (Dh)\nabla u \rangle = \langle \nu, \nabla_{\nabla u}\, h \rangle \\ &= \langle \nu, \nabla_{\nabla u}\, \mathrm{P}h \rangle + \langle \nu, \nabla_{\nabla u}\, (h^\nu \nu) \rangle\,. \end{aligned}$$

Applying $\nabla_{\nabla u}$ to $\langle \mathrm{P}h, \nu \rangle = 0$ yields

$$\langle \nabla_{\nabla u}\, \mathrm{P}h, \nu \rangle = -\langle \mathrm{P}h, \nabla_{\nabla u}\, \nu \rangle = -\langle \mathrm{P}h, L\nabla u \rangle = -\langle L\mathrm{P}h, \nabla u \rangle\,,$$

and applying $\nabla_{\nabla u}$ to $\langle \nu, \nu \rangle = 1$ gives

$$\langle \nu, \nabla_{\nabla u} (h^\nu \nu) \rangle = \nabla_{\nabla u} h^\nu + h^\nu \langle \nu, \nabla_{\nabla u} \nu \rangle = \langle \nabla h^\nu, \nabla u \rangle .$$

We have proved that

$$- \langle \tilde{\nu}'(\underline{h}), \nabla u \rangle = \langle \operatorname{Grad} h^\nu - L\mathrm{P}h, \nabla u \rangle .$$

Putting everything together gives the assertion. ■

(1.43) is also valid for $m = 2$ with almost the same proof.

1.4. On the null-space of the first derivatives

Lemma 1.25. *Let K be a C^2 smooth, sound-soft scatterer, and u_{i} an incident field that does* not *satisfy the radiation condition (0.4). Then*

$$u'_\infty(h) = 0 \Longleftrightarrow h \cdot \nu = 0. \tag{1.44}$$

Proof. If $h \cdot \nu = 0$, then $u'(h)|_{\partial K} = -\frac{\partial u}{\partial \nu}(h \cdot \nu) = 0$, and hence $u'_\infty(h) = 0$ by the uniqueness of the exterior Dirichlet problem.

Assume that $u'_\infty(h) = 0$. Then, by Rellich's lemma (cf., e.g., [CK97, Lemma 2.11]), $u'(h) = 0$ in ${}^cK$, so in particular $\frac{\partial u}{\partial \nu}(h \cdot \nu) = 0$ on dK. Assume that $(h \cdot \nu)(x_0) \neq 0$ for some $x_0 \in \partial K$. Then, by continuity, $h \cdot \nu \neq 0$ on some open neighborhood of x_0 on ∂K, hence $\frac{\partial u}{\partial \nu} = 0$ on this neighborhood. As $u|_{\partial K} = 0$, Holmgren's uniqueness theorem (cf., e.g., [RR92]) applies and yields $u = 0$ on ${}^cK$. This contradicts the fact that u_{i} does not satisfy the radiation condition, so our assumption $(h \cdot \nu)(x_0) \neq 0$ was false. ■

For sound-hard obstacles the above argument cannot be applied. In fact, the following example from [Hoh98] shows that (1.44) does not hold for general u_{i}.

Assume that $K \subset \mathbb{R}^2$ is the unit disk, $\kappa \in \mathbb{N}$, and $u_{\mathrm{i}}(r, t) = J_\kappa(\kappa r) \mathrm{e}^{\mathrm{i}\kappa t}$ in polar coordinates. Note that due to the integral representation of Bessel functions (cf., e.g., [Kre89, (18.22)]), u_{i} is a superposition of plane waves:

$$u_{\mathrm{i}}(x) = \frac{\mathrm{i}^\kappa}{2\pi} \int_0^{2\pi} \mathrm{e}^{\mathrm{i}\kappa \langle x, d(\varphi) \rangle} \mathrm{e}^{\mathrm{i}\kappa\varphi} \, \mathrm{d}\varphi, \qquad d(\varphi) := (-\cos\varphi, -\sin\varphi).$$

We readily compute

$$u_{\mathrm{s}}(r, t) = -\frac{J'(\kappa)}{H_\kappa^{(1)'}(\kappa)} H_\kappa^{(1)}(\kappa r) \mathrm{e}^{\mathrm{i}\kappa t}.$$

For $h = \nu$, the boundary condition (1.43) yields

$$\frac{\partial u'(h)}{\partial \nu} = \frac{\partial^2 u}{\partial t^2} + \kappa^2 u = 0.$$

Hence $u'_\infty(h) = 0$ for $h = \nu$.

It is not known whether or not (1.44) holds for the sound-hard scattering problem if u_i is a plane wave.

1.5. Relation to other results

The idea to use the variational formulations (1.3) and (1.21) in order to establish differentiability of the scattered field has been introduced by Kirsch [Kir93] and Hettlich [Het95, Het98]. They considered the special case of the first derivative for smooth domains. In some sense the proofs are organized in reverse order as compared to ours. The function $\tilde{u}'(h)$ is introduced by $\tilde{u}'(h) := u'(h) + \nabla u \cdot h$ (cf. (1.18)) where $u'(h)$ is defined as the radiating solution to the Helmholtz equation that has the boundary values $u'(h) = -\nabla u \cdot h$ on ∂K. In order to show that $u'(h)$ is the Fréchet derivative of u, the variational equation

$$S'(h)(u, v) = -S(\tilde{u}'(h), v)$$

is established by explicit computation of $S'(h)$ and repeated application of Green's and Gauß' formulae. This approach becomes rather complicated for Neumann boundary conditions and especially for higher derivatives (cf. [HR] where the boundary values of the second derivative with Dirichlet boundary conditions are computed).

In the literature on domain derivatives (cf., e.g., [Sim80, SZ92]), variations of the domain are usually defined by diffeomorphisms between domains, instead of starting with differentiable functions on the boundary and extending these functions to the entire domain. The latter approach has the advantage that one can choose the support of the extended functions, i.e. the domain where the diffeomorphism differs from identity, arbitrarily small. This, together with the ellipticity of the differential equation, makes it possible to obtain higher order Fréchet derivatives in higher norms *arbitrarily close* to the boundary (Theorem 1.9) and to derive eq. (1.18) in *all* of ${}^cK$. If (1.18) was available only up to some fixed distance to the boundary, this would not have any implications for the boundary values of the derivatives.

A different approach based on boundary integral operators has been introduced by Potthast [Pot94, Pot96b]. It is shown for C^2-smooth boundaries that the scattered field depends C^∞ on the boundary with respect to the C^2-norm. The derivation of the boundary conditions has been simplified in [HS98]. The integral equation approach has the interesting feature that it yields an alternative implementable formula for the derivative of the scattered field that does not contain its boundary values (cf. Moench [Mön96, Mön97]). However, as discussed in [Hoh98], the numerical method described here is more efficient. A disadvantage of the integral equation approach consists in the high regularity assumptions for the boundary. Moreover, although the boundary values of the second derivative for Dirichlet boundary conditions can be derived quite easily with the methods in [HS98], general formulas as in Theorems 1.12 and 1.19, which comes out naturally from our approach, seem hard to reach.

2. Numerical computation of Fréchet derivatives

We have seen in Chapter 1 that Fréchet derivatives of solutions to scattering problems are characterized by the same type of boundary value problem as the solutions itself, and we have determined the boundary values. Therefore, the derivatives can be computed by solving boundary value problems of the same type as that of the solution. The boundary values of the Fréchet derivatives involve the unknown Cauchy data which are solutions of certain integral equations. For Dirichlet boundary conditions this has been used in [Kre94] to compute the first Fréchet derivative. For other boundary conditions and higher order derivatives the main difficulty is to compute tangential derivatives of the unknown Cauchy data which are given as an approximate solution of an integral equation. We describe an approach where the approximate solution is a trigonometric polynomial, that thus differentiation can be carried out exactly. Moreover, we provide an error analysis in Sobolev spaces that justifies this differentiation. Finally, we compare our method of computing tangential derivatives to a different approach suggested by Schwab and Wendland.

2.1. Boundary integral equations

In this section we briefly describe the integral equation approaches that is used in the following to solve acoustic obstacle scattering problems. We assume the reader to be familiar with the basic concepts of integral equation methods and refer to [CK83, CK97, Kre89] for introductory texts.

As opposed to our more general theoretical investigations in Chapter 1, we now additionally assume that $m = 2$, that the scatterer K is connected, and that ∂K is at least C^2-smooth.

Let us start with the sound soft scattering problem (0.1), (0.4) with classical boundary condition $u|_{\partial K} = 0$ where $u \in C^2({}^cK) \cap C(\overline{{}^cK})$. We describe two methods to solve this problem, and both are used in Section 2.5.. The first starts from the mixed layer potential ansatz

$$u_{\mathrm{s}}(x) = \int_{\partial K} \left\{ \frac{\partial \Phi(x,y)}{\partial \nu(y)} - \mathrm{i}\eta\Phi(x,y) \right\} \varphi(y)\,\mathrm{d}s(y), \qquad x \in {}^{c}K \tag{2.1}$$

with density $\varphi \in C(\partial K)$ and a real coupling parameter $\eta \neq 0$. Here

$$\Phi(x,y) := \frac{i}{4} H_0^{(1)}(\kappa|x-y|), \qquad x \neq y, \tag{2.2}$$

is the fundamental solution to the Helmholtz equation in $\mathbb{R}^2$, and $H_0^{(1)}$ is the Hankel function of the first kind of order 0. The ansatz (2.1) avoids the non-uniqueness of the interior Neumann problem for certain wave numbers κ which poses a problem for the double layer potential ansatz $\eta = 0$.

By the jump relations, u_{s} given by (2.1) solves the Dirichlet problem (0.1), (0.4) with boundary condition $u_{\mathrm{s}}|_{\partial K} = f$, $f \in C(\partial K)$, if the density φ solves the integral equation

$$\varphi + D\varphi - i\eta S\varphi = 2f \tag{2.3}$$

on ∂K. Here the single layer potential operator S and the double layer potential D are defined by

$$\begin{aligned} (S\varphi)(x) &:= 2\int_{\partial K} \Phi(x,y)\varphi(y)\,\mathrm{d}s(y), \\ (D\varphi)(x) &:= 2\int_{\partial K} \frac{\partial \Phi(x,y)}{\partial \nu(y)}\varphi(y)\,\mathrm{d}s(y). \end{aligned}$$

It can be shown that the operators $S, D : C(\partial K) \to C(\partial K)$ are compact, and that the homogeneous equation (2.3) only has the solution $\varphi = 0$. Hence, by Riesz theory, (2.3) has a unique solution for all right hand sides $f \in C(\partial K)$.

In addition to the mixed layer potential ansatz, we also need a Green's ansatz which yields $\frac{\partial u}{\partial \nu}$ as solution of an integral equation that is adjoint to (2.3) (cf. [Kre94]). We start from Green's representation formula

$$u_{\mathrm{s}}(x) = \int_{\partial K} \left\{ u_{\mathrm{s}}(y)\frac{\partial \Phi(x,y)}{\partial \nu(y)} - \frac{\partial u_{\mathrm{s}}(y)}{\partial \nu}\Phi(x,y) \right\} ds(y), \qquad x \in {}^{c}K$$

and add the formula

$$0 = \int_{\partial K} \left\{ u_{\mathrm{i}}(y)\frac{\partial \Phi(x,y)}{\partial \nu(y)} - \frac{\partial u_{\mathrm{i}}(y)}{\partial \nu}\Phi(x,y) \right\} ds(y), \qquad x \in {}^{c}K$$

which is Green's Second Theorem in K for $\Phi(x,\cdot)$ and u_{i}. This yields

$$u_{\mathrm{s}}(x) = \int_{\partial K} \left\{ u(y)\frac{\partial \Phi(x,y)}{\partial \nu(y)} - \frac{\partial u(y)}{\partial \nu}\Phi(x,y) \right\} ds(y), \qquad x \in {}^{c}K, \tag{2.4}$$

and for $u = 0$ on ∂K this reduces to

$$u(x) + \int_{\partial K} \frac{\partial u(y)}{\partial \nu} \Phi(x, y)\, ds(y) = u_{\mathrm{i}}(x), \qquad x \in {}^cK.$$

Letting x tend to ∂K and taking the normal derivative in this equation yields

$$\frac{1}{2} S \frac{\partial u}{\partial \nu} = u_{\mathrm{i}} \quad \text{and} \quad \frac{1}{2}(I + D') \frac{\partial u}{\partial \nu} = \frac{\partial u_{\mathrm{i}}}{\partial \nu},$$

rsp. Here the normal derivative of the single layer potential

$$(D'\varphi)(x) := 2 \int_{\partial K} \frac{\partial \Phi(x, y)}{\partial \nu(x)} \varphi(y)\, \mathrm{d}s(y),$$

is adjoint to D with respect to the bilinear system $\langle \varphi_1, \varphi_2 \rangle := \int_{\partial K} \varphi_1 \varphi_2 \, \mathrm{d}s$. Now, by linear combination, we obtain the integral equation

$$(I + D' - \mathrm{i}\eta S) \frac{\partial u}{\partial \nu} = 2 \frac{\partial u_{\mathrm{i}}}{\partial \nu} - 2\mathrm{i}\eta u_{\mathrm{i}} \tag{2.5}$$

announced above.

Now, we turn to the problem (0.1), (0.4) with Neumann boundary condition $\frac{\partial u_{\mathrm{s}}}{\partial \nu} = g$ where the boundary data are in the Hölder space $C^{0,\alpha}(\partial K)$, $0 < \alpha < 1$. Here the ansatz (2.1) leads to the integral equation

$$T\varphi - \mathrm{i}\eta D'\varphi + \mathrm{i}\eta\varphi = 2g \tag{2.6}$$

with the normal derivative of the double layer potential defined by

$$(T\varphi)(x) := 2 \frac{\partial}{\partial \nu(x)} \int_{\partial K} \frac{\partial \Phi(x, y)}{\partial \nu(y)} \varphi(y)\, \mathrm{d}s(y).$$

It can be shown that (2.6) has a unique solution $\varphi \in C^{1,\alpha}(\partial K)$ for all right hand sides $g \in C^{0,\alpha}(\partial K)$, and we briefly sketch how this can be accomplished with help of the Riesz-Fredholm theory as presented in [Kre89, Chapter 5]. The operator T is bounded from $C^{1,\alpha}(\partial K)$ to $C^{0,\alpha}(\partial K)$, and $-\mathrm{i}\eta D' + \mathrm{i}\eta I$ is compact in these function spaces. By the identities $ST = -I + D^2$ and $TS = -I + D'^2$, the operator $S : C^{0,\alpha}(\partial K) \to C^{1,\alpha}(\partial K)$ is a regularizer of $A := T - \mathrm{i}\eta D' + \mathrm{i}\eta I$. Moreover, the adjoint with respect to the bilinear systems defined by $\langle \varphi_1, \varphi_2 \rangle := \int_{\partial K} \varphi_1 \varphi_2 \, \mathrm{d}s$ is $A' = T - \mathrm{i}\eta D' + \mathrm{i}\eta I \in L(C^{1,\alpha}(\partial K), C^{0,\alpha}(\partial K))$. We have $\operatorname{ind} A = \operatorname{ind} A + \operatorname{ind} S = \operatorname{ind} AS = 0$ as $S = S'$. Hence, existence of a solution to (2.6) follows from uniqueness, and uniqueness can be shown by standard arguments.

Finally, we also describe Green's ansatz for the sound hard scattering problem. With $\frac{\partial u}{\partial \nu} = 0$ on ∂K, (2.4) reduces to

$$\int_{\partial K} \frac{\partial \Phi(x,y)}{\partial \nu(y)} u(y)\, \mathrm{d}s(y) - u(x) = -u_{\mathrm{i}}(x), \qquad x \in {}^cK,$$

and taking the boundary values and the normal derivative yields

$$\frac{1}{2}(D - I)u = -u_{\mathrm{i}} \quad \text{and} \quad \frac{1}{2}Tu = -\frac{\partial u_{\mathrm{i}}}{\partial \nu},$$

rsp. Thus we arrive at the integral equation

$$(T - \mathrm{i}\eta D + \mathrm{i}\eta I)u = -2\frac{\partial u_{\mathrm{i}}}{\partial \nu} + 2\mathrm{i}\eta u_{\mathrm{i}}, \tag{2.7}$$

which is adjoint to (2.6).

2.2. Discretization of the boundary integral equations

After parameterizing the boundary curve by a smooth, 2π-periodic function z, the boundary integral equations (2.3) and (2.6) can be transformed to integral equations for 2π-periodic functions. Whereas (2.3) is of the standard form "I+compact", the numerical solution of (2.6) poses some problems due to the singular integral operator T. We are going to adopt a method that has originally been developed by Kress and Sloan [KS93] to solve an integral equation of the first kind. After splitting off the singularities in the kernels, the integral operators are replaced by quadrature operators based on trigonometric interpolation. Thus, in the case of integral equations of the second kind, our method is similar to Nyström's method, and, in fact, the finite dimensional systems for both methods coincide. However, to obtain the approximate solution from the nodal values, we do not use Nyström interpolation, but trigonometric interpolation. This will be important in Section 2.5. as it allows exact differentiation of the approximate solutions. In Section 2.3. we justify this differentiation by providing an error analysis in Sobolev spaces of arbitrary order, extending results in [KS93]. For a different analysis of (2.6) in a Hölder space setting, we refer to Kress [Kre95c] and Hohage [Hoh98]. Our presentation follows a paper by Hohage and Schormann [HS98] where the method has been applied to a system of integral equations arising in a transmission problem.

Parametrization. With a slight abuse of notation, we denote boundary integral operators and their parametrized versions by the same letters. It turns out that adjoint boundary integral operators lead to adjoint parametrized operators if we incorporate an additional factor $|z'(t)|$. E.g., our parametrized version of the single layer potential operator is

$$(S\psi)(t) = \frac{\mathrm{i}}{2}\int_0^{2\pi} H_0^{(1)}(\kappa|z(t)-z(\tau)|)|z'(t)||z'(\tau)|\psi(\tau)\,\mathrm{d}\tau, \qquad t\in[0,2\pi].$$

Here $\psi(t)=\varphi(z(t))$, and $|z'(\tau)|\,\mathrm{d}\tau$ corresponds to the arc-length element $\mathrm{d}s$. Note that S is self-adjoint due to the additional factor $|z'(t)|$.

Let us now describe how the singularities of the kernels of are split off. All of the (parametrized) boundary integral operators S, D, D', T can be decomposed into components of the following form:

$$(B_1(k)\psi)(t) := \int_0^{2\pi} k(t,\tau)\ln\left(4\sin^2\frac{t-\tau}{2}\right)\psi(\tau)\,\mathrm{d}\tau, \tag{2.8a}$$

$$(B_2(k)\psi)(t) := \int_0^{2\pi} k(t,\tau)\psi(\tau)\,\mathrm{d}\tau, \tag{2.8b}$$

$$(T_0\psi)(t) := \frac{1}{2\pi}\int_0^{2\pi}\cot\frac{\tau-t}{2}\psi'(\tau)\,\mathrm{d}\tau. \tag{2.8c}$$

In case of the Laplace equation ($\kappa=0$) for the unit circle, $B_1(\frac{1}{2\pi})$ corresponds to the single layer potential operator, and T_0 to the normal derivative of the double layer potential. The trigonometric monomials

$$\epsilon_l(\tau) := \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}l\tau}, \qquad l\in\mathbb{Z} \tag{2.9}$$

are eigenfunctions of the operators $B_1(\frac{1}{2\pi})$ and T_0 with eigenvalues

$$B_1(\frac{1}{2\pi})\epsilon_l = \begin{cases} -|l|^{-1}\epsilon_l & l\neq 0\\ 0 & l=0\end{cases} \tag{2.10}$$

$$T_0\epsilon_l = -|l|\epsilon_l, \qquad l\in\mathbb{Z}. \tag{2.11}$$

It can be shown that for general wave numbers $\kappa>0$ there exist kernel functions such that the decompositions

$$S = B_1(k_{S,1}) + B_2(k_{S,2}), \tag{2.12a}$$

$$D = B_1(k_{D,1}) + B_2(k_{D,2}), \tag{2.12b}$$

$$D' = B_1(k_{D',1}) + B_2(k_{D',2}), \tag{2.12c}$$

$$T = T_0 + B_1(k_{T,1}) + B_2(k_{T,2}). \tag{2.12d}$$

hold. All kernel functions are periodic in both variables and (roughly) as smooth as the parametrization. For more information on the kernel functions and explicit formulae, we refer to [CK97] and [Kre95c]. Now, the parametrized versions of (2.3) and (2.6) can be written as

$$\psi + B_1(k_1^{\mathrm{D}})\psi + B_2(k_2^{\mathrm{D}})\psi = \tilde{f}, \tag{2.13}$$

$$T_0\psi + B_1(k_1^{\mathrm{N}})\psi + B_2(k_2^{\mathrm{N}})\psi + i\eta|z'|\psi = \tilde{g}, \tag{2.14}$$

rsp. Here $k_j^{\mathrm{D}} := k_{D',j} + \mathrm{i}\eta k_{S,j}$, $k_j^{\mathrm{N}}(t,\tau) := (k_{T,j} - \mathrm{i}\eta k_{D',j})(t,\tau)$ $(j = 1,2)$, $\psi(t) := \varphi \circ z$, $\tilde{f} := 2|z'| \cdot (f \circ z)$, and $\tilde{g} := 2|z'| \cdot (g \circ z)$.

Approximation. Now, we approximate the operators introduced in (2.8a), (2.8b) by quadrature operators based on trigonometric interpolation. Recall that with $n \in \mathbb{N}$ the interpolation problem for the equidistant points

$$t_j^{(n)} := jh, \quad j = 0, \dots, 2n-1, \quad h := \frac{\pi}{n}, \tag{2.15}$$

with respect to the subspace T_n of trigonometric polynomials of the form

$$v(t) = \sum_{l=0}^{n} a_l \cos lt + \sum_{l=1}^{n-1} b_l \sin lt \tag{2.16}$$

is uniquely solvable and defines an interpolation operator $P_n : C([0,2\pi]) \to T_n$. With the Lagrange functions

$$L_j^{(n)}(t) := \frac{1}{2n}\left(1 + 2\sum_{m=1}^{n-1} \cos m(t - t_j^{(n)}) + \cos n(t - t_j^{(n)})\right), \tag{2.17}$$

the operator P_n can be written as

$$(P_n\psi)(t) = \sum_{j=0}^{2n-1} \psi(t_j^{(n)}) L_j^{(n)}(t). \tag{2.18}$$

We introduce the quadrature operators

$$\begin{aligned} (B_{1,n}(k)\psi)(t) &:= \int_0^{2\pi} \ln\left(4\sin^2\frac{t-\tau}{2}\right) P_n\left(k(t,\cdot)\psi\right)(\tau)\,\mathrm{d}\tau, \\ (B_{2,n}(k)\psi)(t) &:= \int_0^{2\pi} P_n\left(k(t,\cdot)\psi\right)(\tau)\,\mathrm{d}\tau, \end{aligned}$$

and approximate (2.13) and (2.14) by

$$\psi_n + P_nB_{1,n}(k_1^{\mathrm{D}})\psi_n + P_nB_{2,n}(k_2^{\mathrm{D}})\psi_n = P_n\tilde{f}, \tag{2.19}$$

$$T_0\psi_n + P_nB_1(k_1^{\mathrm{N}})\psi_n + P_nB_2(k_2^{\mathrm{N}})\psi_n + P_n(i\eta|z'|\psi_n) = P_n\tilde{g}, \tag{2.20}$$

rsp. An important property of these equations is that any solution automatically belongs to $T_n = \operatorname{ran}(P_n)$. This is obvious for (2.19). By virtue of (2.11), it is also true for (2.20).

Finite dimensional system. To arrive at a finite dimensional system equivalent to (2.19) and (2.20), rsp., we need the formulae

$$\begin{aligned}\int_0^{2\pi} \ln\left(4\sin^2\frac{t-\tau}{2}\right)(P_n\psi)(\tau)\,\mathrm{d}\tau &= \sum_{j=0}^{2n-1} R_j^{(n)}(t)\psi(t_j^{(n)}),\\ \int_0^{2\pi}(P_n\psi)(\tau)\,\mathrm{d}\tau &= \frac{\pi}{n}\sum_{j=0}^{2n-1}\psi(t_j^{(n)}),\\ \frac{1}{2\pi}\int_0^{2\pi}\cot\frac{\tau-t}{2}(P_n\psi)'(\tau)\,\mathrm{d}\tau &= \sum_{j=0}^{2n-1} T_j^{(n)}(t)\psi(t_j^{(n)})\end{aligned}$$

with quadrature weights

$$\begin{aligned}R_j^{(n)}(t) &:= -\frac{2\pi}{n}\sum_{m=1}^{n-1}\frac{1}{m}\cos m(t-t_j^{(n)}) - \frac{\pi}{n^2}\cos n(t-t_j^{(n)}),\\ T_j^{(n)}(t) &:= -\frac{1}{n}\sum_{m=1}^{n-1} m\cos m(t-t_j^{(n)}) - \frac{1}{2}\cos n(t-t_j^{(n)})\end{aligned}$$

which can be derived from (2.10), (2.11), and (2.18). Evaluating (2.19) and (2.20) at the points $t_l^{(n)}$, we obtain the following systems of linear equations

$$\begin{aligned}&\psi_n(t_l^{(n)}) + \sum_{j=0}^{2n-1}\left\{R_j^{(n)}(t_l^{(n)})k_1^{\mathrm{D}}(t_l^{(n)},t_j^{(n)}) + \frac{\pi}{n}k_2^{\mathrm{D}}(t_l^{(n)},t_j^{(n)})\right\}\psi_n(t_j^{(n)})\\ &\qquad = \tilde{f}(t_l^{(n)}), \qquad l = 0,\dots,2n-1 \qquad (2.21)\\ &\sum_{j=0}^{2n-1}\left\{T_j^{(n)}(t_l^{(n)}) + R_j^{(n)}(t_l^{(n)})k_1^{\mathrm{N}}(t_l^{(n)},t_j^{(n)}) + \frac{\pi}{n}k_2^{\mathrm{N}}(t_l^{(n)},t_j^{(n)})\right\}\psi_n(t_j^{(n)})\\ &\qquad +\mathrm{i}\eta|z'(t_l^{(n)})|\psi_n(t_l^{(n)}) = \tilde{g}(t_l^{(n)}), \qquad l = 0,\dots,2n-1. \qquad (2.22)\end{aligned}$$

Since the trigonometric polynomials ψ_n are uniquely determined by the nodal values $\psi_n(t_j^{(n)})$, (2.21) is equivalent to (2.19), and (2.22) to (2.20).

2.3. A convergence analysis in Sobolev spaces

In this section we provide an error analysis for the method introduced in Section 2.2.. In the following, let $H^q = H^q([0,2\pi])$ be the Sobolev space of index $q \in \mathbb{R}$ of periodic functions $\psi : [0, 2\pi] \to \mathbb{C}$, equipped with the norm

$$\|\psi\|_q := \left(\sum_{l \in \mathbb{Z}} (1 + l^2)^q |\langle \psi, \epsilon_l \rangle|^2 \right)^{1/2} .$$

We consider the following setup. Let L be a linear operator satisfying

$$L\epsilon_l = c_l \epsilon_l, \qquad l \in \mathbb{Z}$$

for the trigonometric monomials defined in (2.9), and assume that there are constants $\beta \in \mathbb{R}$ and $0 < \gamma_0 \leq \gamma_1$ such that the eigenvalues $c_l \in \mathbb{C}$ satisfy $c_l = c_{-l}$ and

$$\gamma_0 (1 + l^2)^\beta \leq |c_l|^2 \leq \gamma_1 (1 + l^2)^\beta, \qquad l \in \mathbb{Z}. \tag{2.23}$$

Then L is a bounded and boundedly invertible operator from H^q to $H^{q-\beta}$ for all $q \in \mathbb{R}$, and the spaces T_l of trigonometric polynomials introduced in Section 2.2. are invariant under L. Moreover, we consider an operator

$$A \in L(H^{q-\alpha}, H^{q-\beta}) \tag{2.24}$$

with some $\alpha > 0$. Assume that the equation

$$L\psi + A\psi = f \tag{2.25}$$

has only the trivial solution $\psi = 0$ for $f = 0$. Then, by Riesz theory and the compactness of the embedding $H^q \hookrightarrow H^{q-\alpha}$, (2.25) has a unique solution $\psi \in H^q$ for all $f \in H^{q-\beta}$.

The equations (2.13) and (2.14) fit into this abstract framework as follows: In case of (2.13) we have $L = I$, $\beta = 0$, and $A = B_1(k_1^{\mathrm{D}}) + B_2(k_2^{\mathrm{D}})$. For (2.14) we choose $L = T_0 - B_0$, $\beta = 1$. The operator $(B_0\psi)(t) := (2\pi)^{-1} \int_0^{2\pi} \psi \, \mathrm{d}\tau$ is introduced to meet (2.23) for $l = 0$ (cf. (2.11)). Then $A\psi = B_1(k_1^{\mathrm{N}})\psi + B_2(k_2^{\mathrm{N}} + \frac{1}{2\pi})\psi + i\eta|z'|\psi$. In our general setting, the approximations (2.19) and (2.20) to (2.13) and (2.14), rsp., are described by

$$L\psi_n + P_n A_n \psi_n = P_n f. \tag{2.26}$$

The following convergence result has been established in [KS93]. Although we state it with slightly different quantifiers in order to make it more easily and generally applicable in the following, the proof remains almost the same, so we do not repeat it here.

Theorem 2.1. *Let the numbers* $r, p \in \mathbb{R}$ *satisfy* $\max\{\alpha, \beta\} \leq r \leq p$ *and* $p > \max\{\alpha, \beta\} + \frac{1}{2}$, *and assume that (2.24) holds for all* $q \in [r, p]$. *Moreover, let* A_n *be a sequence of operators approximating* A *such that for all* $q \in [r, p]$ *there exists a constant* $c > 0$ *such that*

$$\|(A - A_n)\psi\|_{q-\beta} \leq ch^{p-q}\|\psi\|_{p-\alpha} \tag{2.27}$$

for all $\psi \in T_n$. *Then, for sufficiently large* n *and for all* $f \in H^{p-\beta}$, *there exists a unique solution* $u_n \in T_n$ *to (2.26) satisfying the error estimate*

$$\|\psi - \psi_n\|_q \leq ch^{p-q}\|\psi\|_p \tag{2.28}$$

for all $q \in [r, p]$ *and some constant* c *independent of* f *and* n.

We want to apply this convergence theorem to (2.19) and (2.20) with the specifications $r = 1$ and $\alpha \in (0, \frac{1}{2})$. It remains to verify the conditions (2.24) and (2.27). A crucial tool will be the following estimate on the trigonometric interpolation error

$$\|P_n\psi - \psi\|_q \leq ch^{p-q}\|\psi\|_p \tag{2.29}$$

which holds for all $\psi \in H^p$, $0 \leq q \leq p$, $p > \frac{1}{2}$, and some constant c independent of ψ and n (cf. [KS93, Theorem 2.1]).

An immediate consequence of (2.29) is

$$\|P_n(i\eta|z'|\psi) - i\eta|z'|\psi\|_{q-1} \leq ch^{p-q}\||z'|\psi\|_{p-1} \leq ch^{p-q}\|\psi\|_{p-\alpha}$$

for $z \in C^{p-1}$ and $p \geq 2$, i.e. this part of A_n in (2.20) does satisfy the condition (2.27). Obviously the multiplication operator $\psi \mapsto i\eta|z'|\psi$ also satisfies the condition (2.24). Moreover, it has already been shown in [KS93] that the operators $B_2(k)$ and $B_{2,n}(k)$ satisfy (2.24) and (2.27) for smooth k. Thus, it remains to consider the operators $B_1(k)$ and $B_{1,n}(k)$. In the following proposition we only consider the case $\beta = 0$ since this obviously implies the case $\beta = 1$ needed for (2.14), (2.20).

Proposition 2.2. *Let* $k \in C^p([0, 2\pi]^2)$, $p \in \mathbb{N}$, *be periodic in both variables and* $0 \leq \alpha < \frac{1}{2}$. *Then, for all* $q \in [\alpha, p]$, *the operators* $B_1(k)$ *and* $B_{1,n}(k)$: $H^{q-\alpha} \to H^q$ *are bounded, and the asymptotic estimate*

$$\|B_1(k)\psi - B_{1,n}(k)\psi\|_q \leq ch^{p-q}\|\psi\|_{p-\alpha} \tag{2.30}$$

holds for all $q \in [1, p]$, $\psi \in T_n$ *with some constant* c *independent of* ψ *and* n.

Proof. We first consider $q \in \{1, 2, \ldots, p\}$ and compute the qth derivative of $B_1(k)\psi$ for $\psi \in C^\infty([0, 2\pi])$. Substituting $\tau = \bar\tau + t$ and using periodicity, we obtain

$$\begin{aligned}\frac{d^q}{dt^q}(B_1(k)\psi)(t) &= \frac{d^q}{dt^q}\int_0^{2\pi} \ln\left(4\sin^2\frac{\bar\tau}{2}\right) k(t, \bar\tau + t)\psi(\bar\tau + t)\, \mathrm{d}\bar\tau \\ &= \int_0^{2\pi} \ln\left(4\sin^2\frac{\bar\tau}{2}\right) \frac{\partial^q}{\partial t^q}\Big(k(t, \bar\tau + t)\psi(\bar\tau + t)\Big)\, \mathrm{d}\bar\tau\end{aligned}$$

by a standard corollary to Lebesgue's dominated convergence theorem. Applying the product rule and substituting back yields

$$\frac{d^q}{dt^q}(B_1(k)\psi)(t) = \sum_{\nu=0}^{q}\binom{q}{\nu}\int_0^{2\pi} \ln\left(4\sin^2\frac{t-\tau}{2}\right) \frac{\partial^q}{\partial t^\nu \partial\tau^{q-\nu}}\Big(k(t,\tau)\psi(\tau)\Big)\, \mathrm{d}\tau.$$

Proceeding as above and using

$$\frac{\partial}{\partial t}P_n(k(t,\cdot)\psi) = P_n\Big(\frac{\partial}{\partial t}k(t,\cdot)\psi\Big),$$

which follows immediately from the Lagrange representation of $P_n(k(t,\cdot)\psi)$, we find

$$\begin{aligned}&\frac{d^q}{dt^q}(B_1(k)\psi - B_{1,n}(k)\psi)(t) \\ &= \sum_{\nu=0}^{q}\binom{q}{\nu}\int_0^{2\pi} \ln\left(4\sin^2\frac{t-\tau}{2}\right) \frac{\partial^{q-\nu}}{\partial\tau^{q-\nu}}\Big(I - P_n\Big)\left(\frac{\partial^\nu}{\partial t^\nu}k(t,\cdot)\psi\right)(\tau)\, \mathrm{d}\tau.\end{aligned}$$

Hence, by (2.10), we obtain

$$\frac{d^q}{dt^q}(B_1(k)\psi - B_{1,n}(k)\psi)(t) = \sum_{\nu=0}^{q}\binom{q}{\nu}\sum_{l\in\mathbb{Z}}\gamma_l a^l_{\nu,q}(t)\epsilon_l(t)$$

with the Fourier coefficients

$$a^l_{\nu,q}(t) := \left\langle \frac{\partial^{q-\nu}}{\partial\tau^{q-\nu}}\Big(I - P_n\Big)\left(\frac{\partial^\nu}{\partial t^\nu}k(t,\cdot)\psi\right), \epsilon_l \right\rangle.$$

Here interchanging summation and integration is justified by Lebesgue's dominated convergence theorem and uniform convergence of the Fourier series of C^1-functions. Under the given restrictions on s, q and α the estimate

(2.29) implies that

$$\begin{aligned}\left\|\frac{\partial^{q-\nu}}{\partial\tau^{q-\nu}}\Big(I-P_n\Big)\left(\frac{\partial^\nu}{\partial t^\nu}k(t,\cdot)\psi\right)\right\|_{-\alpha} &\le c\left\|\Big(I-P_n\Big)\left(\frac{\partial^\nu}{\partial t^\nu}k(t,\cdot)\psi\right)\right\|_{q-\alpha}\\ &\le ch^{p-q}\left\|\frac{\partial^\nu}{\partial t^\nu}k(t,\cdot)\psi\right\|_{p-\alpha}\\ &\le ch^{p-q}\|\psi\|_{p-\alpha}.\end{aligned}$$

It follows by the Cauchy-Schwarz inequality and the fact that $\sum_{l\in\mathsf{Z}}\gamma_l^2(1+l^2)^\alpha<\infty$ for $\alpha<\frac{1}{2}$ that

$$\begin{aligned}&\left|\frac{d^q}{dt^q}(B_1(k)\psi-B_{1,n}(k)\psi)(t)\right|^2\\ &\quad\le\left(\sum_{\nu=0}^{q}\binom{q}{\nu}^2\sum_{l\in\mathsf{Z}}\frac{\gamma_l^2(1+l^2)^\alpha}{2\pi}\right)\left(\sum_{\nu=0}^{q}\sum_{l\in\mathsf{Z}}\frac{|a_{\nu,q}^l(t)|^2}{(1+l^2)^\alpha}\right)\\ &\quad\le c\sum_{\nu=0}^{q}\left\|\frac{\partial^{q-\nu}}{\partial\tau^{q-\nu}}(I-P_n)\left(\frac{\partial^\nu}{\partial t^\nu}k(t,\cdot)\psi\right)\right\|_{-\alpha}^2\le c\Big(h^{p-q}\|\psi\|_{p-\alpha}\Big)^2.\end{aligned}$$

Integrating this inequality over $[0,2\pi]$ yields

$$\begin{aligned}\Big\|B_1(k)\psi-B_{1,n}(k)\psi\Big\|_q^2 &\le c\int_0^{2\pi}\left(\left|\frac{d^q}{dt^q}(B_1(k)\psi-B_{1,n}(k)\psi)(t)\right|^2+\right.\\ &\qquad\left.+\Big|(B_1(k)\psi-B_{1,n}(k)\psi)(t)\Big|^2\right)\mathrm{d}t\\ &\le c\left(h^{p-q}\|\psi\|_{p-\alpha}\right)^2.\end{aligned}$$

Hence we have established (2.30) for $q\in[1,p]\cap\mathbb{N}$ and $\psi\in C^\infty$. This result can now be extended to all $\psi\in H^{p-\alpha}$ by approximation and to all $q\in[1,p]$ by interpolation.

For $q=p$ the estimate (2.30) implies boundedness of $B_1(k)-B_{1,n}(k)$: $H^{p-\alpha}\to H^p$. Boundedness of $B_1(k),B_{1,n}(k):H^{q-\alpha}\to H^q$ for $q\in[\alpha,p]$ is shown analogously. ■

We have shown that all assumptions of Theorem 2.1 are satisfied for the integral equations (2.13), (2.14) and their discretized versions (2.19) and (2.20) if the parametrization z of the boundary is sufficiently smooth. Therefore the error estimate (2.28) holds. In particular derivatives $\psi_n^{(\nu)}$ of the approximate solutions converge to derivatives $\psi^{(\nu)}$ of the exact solution, and these derivatives can easily be computed by an FFT algorithm (cf. p. 118) since ψ_n is a trigonometric polynomial.

2.4. The method of Schwab and Wendland

A different method to compute derivatives of a solution ψ to an integral equation

$$A\psi = f$$

has been suggested by Schwab and Wendland and is described for integral equations on closed surfaces in [SW] and for closed curves in [SSW96]. We will consider the latter case. If A is a pseudodifferential operator on a closed curve, the following commutators with the arc-length derivative ∂_s are well defined

$$A_{(0)} := A, \qquad A_{(j)} := \partial_s A_{(j+1)} - A_{(j)}\partial_s.$$

The essential point is that these commutators are again integral operators of the same order as A, and the kernels can be computed explicitly. For some boundary integral operators for the Helmholtz equations such commutators have been expressed in terms of other commonly used boundary integral operators by Kirsch [Kir84, Kir89b].

An induction argument shows that

$$\partial_s^k A\psi = \sum_{j=0}^{k} \binom{k}{j} A_{(j)} \partial_s^{(k-j)} \psi, \qquad k \in \mathbb{N}.$$

This leads to the following triangular system of equations to compute $\partial_s^l \psi$

$$\begin{aligned} A\psi &= f \\ A\partial_s^k \psi &= \partial_s^k f - \sum_{j=1}^{k} \binom{k}{j} A_{(j)} \partial_s^{k-j} \psi, \qquad k = 1, 2, \ldots, l. \end{aligned}$$

Note that only the operator A has to be inverted.

We mention that this method has actually been devised for quite a different purpose, namely to evaluate potentials near the boundary in integral equation methods for partial differential equations. A straightforward evaluation of the potential operators does not yield satisfactory results due to the singularity of the kernels. Much better results are obtained by a Taylor expansion on the boundary. The higher order normal derivatives needed there can be expressed in terms of tangential derivatives, and to compute those the above method was needed.

We would like to compare the merits of both approaches to compute tangential derivatives. The method described in Sections 2.2. and 2.3. has the advantage that it can easily be implemented and yields highly accurate results for smooth data. The additional work to obtain tangential derivatives amounts to computing derivatives of trigonometric polynomials. For the method of Schwab and Wendland on the other hand, matrices for the commutators have to be implemented and computed, and the right hand side has to be differentiated.

The method of Schwab and Wendland has the advantage that it is more generally applicable. In particular, it can be used for three-dimensional problems although no numerical examples have been reported for this case, yet. It is claimed that the method can also be applied to piecewise analytic curves with corners, but to our knowledge the details still have to be carried out.

2.5. A numerical example

Our numerical example is concerned with the computation of the first Fréchet derivative with Neumann boundary conditions. The parametrized version of the integral equation (2.7) is

$$T_0 u + B_1(k_1^{\mathrm{N},t})u + B_2(k_2^{\mathrm{N},t})u + i\eta|z'|u = w \tag{2.31}$$

with $k_j^{\mathrm{N},t}(t,\tau) := k_j^{\mathrm{N}}(\tau,t)$, $(j=1,2)$ and $w := -2|z'|(\frac{\partial u_{\mathrm{i}}}{\partial \nu} - \mathrm{i}\eta u_{\mathrm{i}})$. If (2.22) is written as $M\underline{\psi}_n = \underline{g}$, then (2.31) leads to the transposed system

$$M^t \underline{u}_n = \underline{w} \tag{2.32}$$

since both $R_j^{(n)}(t_l^{(n)})$ and $T_j^{(n)}(t_l^{(n)})$ only depend on $|j-l|$ and n. Note that to solve both (2.22) and (2.32) only one LR-decomposition has to be computed.

Let us summarize our algorithm:

1. Solve (2.32) to find an approximate solution u_n to (2.31).
2. Evaluate the first and second derivatives of the trigonometric polynomial u_n (cf. p. 118) and compute the right hand side of (1.43).
3. Compute the function $u'(h)$ with a potential ansatz, i.e. solve (2.22) with the right hand side calculated in step 2. Use the LR-decomposition from step 1.

If in the context of a Newton method the operator has to be evaluated as well as the derivative, u_n can be used to compute u_s and u_∞ without much additional effort (cf. (2.4)).

Example 2.3. The function

$$z(t) := \frac{1 + 0.9\cos t + 0.1\sin t}{1 + 0.75\cos t} \begin{pmatrix} \cos t \\ \sin t \end{pmatrix}$$

describes a bean-shaped domain in $\mathbb{R}^2$. We choose $\kappa = 1$, $d = (0, 1)$ and $h(t) = \sin 3t \begin{pmatrix} \cos t \\ \sin t \end{pmatrix}$, and calculate the function $u'_\infty(h)$ at the points d and $-d$ for different values of the discretization level n (Table 2.1). Fast convergence is clearly exhibited.

n	$\mathrm{Re}\, v_\infty(d)$	$\mathrm{Im}\, v_\infty(d)$	$\mathrm{Re}\, v_\infty(-d)$	$\mathrm{Im}\, v_\infty(-d)$
16	-0.200933478	0.0585250333	-0.0158538563	-0.090990894
32	-0.190544511	0.0796748362	-0.0107629556	-0.147480089
64	-0.190623075	0.0794935566	-0.0108395810	-0.147031877
128	-0.190623075	0.0794935572	-0.0108395803	-0.147031878
256	-0.190623075	0.0794935572	-0.0108395803	-0.147031878

Table 2.1: Convergence of the numerical approximations to the Fréchet derivative $v_\infty = u'_\infty(h)$ for Neumann boundary conditions

3. Regularization of Linear Exponentially Ill-Posed Problems

The accuracy of approximate solutions to ill-posed problems depends on the *degree of ill-posedness* of the problem. Inverse obstacle scattering problems are *severely* of more precisely *exponentially ill-posed*. The classical theory of ill-posed problems which deals with error estimates for approximate solutions given a certain data noise level is only applicable to mildly ill-posed problems. Therefore, there is a need to extend this theory to exponentially ill-posed problems. It turns out that even the linear case has not been investigated sufficiently. Therefore, we first look at convergence rates of regularization methods for linear exponentially ill-posed problems and apply these results to inverse problems in heat conduction and satellite gradiometry. The nonlinear case, which is important for inverse scattering problems, is treated in the next chapter.

3.1. Introduction

In this section we review some basic notions of linear regularization theory following the monograph by Engl, Hanke, Neubauer [EHN96]. Let us consider a linear ill-posed operator equation

$$Tx = y, \qquad y \in \operatorname{ran}(T) \tag{3.1}$$

where $T : X \to Y$ is a bounded linear operator between Hilbert spaces X and Y. (3.1) is called *ill-posed* in the sense of Hadamard if T does not have a bounded inverse $T^{-1} : Y \to X$ defined on all of Y, i.e. if a solution to (3.1) does not exist for all $y \in Y$, or if it fails to be unique, or if it does not depend continuously on the data y. Of these three undesirable properties, the last one is the hardest to deal with, so we are mainly interested in this case. If T is compact and $\dim \operatorname{ran}(T) = \infty$, the degree of ill-posedness is characterized by the rate of decay of the singular values σ_n of T. If $1/\sigma_n = \mathrm{O}(n^\alpha)$ for some

$\alpha > 0$, (3.1) is called *mildly ill-posed*, otherwise it is called *severely ill-posed.* If $1/\sigma_n = \mathrm{O}(\exp(n^\alpha))$ for some $\alpha > 0$, (3.1) is called *exponentially ill-posed.*

We want to find an approximation to the *best approximate solution*

$$x^\dagger := T^\dagger y$$

of (3.1) defined by the Moore-Penrose inverse $T^\dagger$ of T. Recall that $T^\dagger : \mathrm{ran}(T) + \mathrm{ran}(T)^\perp \to X$ is given by $T^\dagger T x = x$ for $x \in N(T)^\perp$ and $T^\dagger y = 0$ for $y \in \mathrm{ran}(T)^\perp$, and that $x^\dagger$ has minimum norm among all solutions to the minimization problem $\|Tx - y\| = \min!$ with $x \in X$. Of course, if T is injective and has dense range, then $T^\dagger$ coincides with the ordinary inverse T^{-1} on its domain $\mathrm{ran}(T)$.

A direct evaluation of the unbounded operator $T^\dagger$ would cause serious stability problems, especially if the available data y^δ are perturbed by noise, which is always the case in practice. We assume that some estimate on the *noise level* δ is known, i.e.

$$\|y^\delta - y\| \le \delta. \tag{3.2}$$

To obtain stable solutions to (3.1), we approximate the unbounded operator $T^\dagger$ by a family of continuous *regularization operators* $R_\alpha : Y \to X$, parametrized by some *regularization parameter* $\alpha \in \mathbb{R}^+$.

Definition 3.1. A family $R_\alpha : Y \to X$ of bounded linear operators together with some *parameter choice rule*

$$\alpha : \{(\delta, y^\delta) \in \mathbb{R}^+ \times Y : \exists y \in \mathrm{ran}(T)\ \|y^\delta - y\| \le \delta\} \to \mathbb{R}^+$$

is called a (linear) *regularization method* for T if

$$\lim_{\alpha \to 0} R_\alpha y = T^\dagger y \qquad \text{for all } y \in \mathrm{ran}(T) \tag{3.3}$$

and if the regularized solutions $x_\alpha^\delta := R_{\alpha(\delta, y^\delta)} y^\delta$ converge to the best approximate solution $x^\dagger$ for all $y \in \mathrm{ran}(T)$ in the following (worst case) sense:

$$\sup\{\|x_\alpha^\delta - x^\dagger\| : \|y^\delta - y\| \le \delta\} \to 0 \quad \text{as } \delta \to 0 \tag{3.4}$$

If α depends only on the noise level δ, we call it an *a-priori* parameter choice rule, otherwise an *a-posteriori* parameter choice rule.

All regularization operators that we consider here can be written in the form

$$R_\alpha := g_\alpha(T^*T)T^* \tag{3.5}$$

	$g_\alpha(\lambda)$	$r_\alpha(\lambda)$
Tikhonov	$\dfrac{1}{\lambda+\alpha}$	$\dfrac{\alpha}{\lambda+\alpha}$
iterated Tikhonov	$\dfrac{(\lambda+\alpha)^l-\alpha^l}{\lambda(\lambda+\alpha)^l}$	$\left(\dfrac{\alpha}{\lambda+\alpha}\right)^l$
TSVD	$\begin{cases} \lambda^{-1}, & \lambda \geq \alpha \\ 0, & \lambda < \alpha \end{cases}$	$\begin{cases} 0, & \lambda \geq \alpha \\ 1, & \lambda < \alpha \end{cases}$
Landweber iteration	$\sum_{j=0}^{k-1}(1-\lambda)^j$	$(1-\lambda)^k$

Table 3.1: Spectral characterization of the regularization methods in Example 3.2

with some function g_α satisfying

$$\lim_{\alpha \searrow 0} g_\alpha(\lambda) = \frac{1}{\lambda} \tag{3.6}$$

for all $\lambda \in \sigma(T^*T)\backslash\{0\}$. Then

$$x^\dagger - x_\alpha = r_\alpha(T^*T)x^\dagger \tag{3.7}$$

with

$$r_\alpha(\lambda) := 1 - \lambda g_\alpha(\lambda) \tag{3.8}$$

and $x_\alpha := R_\alpha y$. The formulae (3.5) and (3.7) have to be understood in the sense of the functional calculus. The reader not familiar with spectral theory may find an introduction in [EHN96] and a more detailed treatment in [HS71].

Table 3.1 lists the functions g_α and r_α for some well known regularization methods. A brief description follows:

Example 3.2. 1. *(Tikhonov regularization)* For $\alpha > 0$, x_α^δ is the unique solution to the operator equation

$$T^*Tx_\alpha^\delta + \alpha x_\alpha^\delta = T^*y^\delta$$

or, equivalently, to the unique minimizer of the *Tikhonov functional*

$$\|Tx - y^\delta\|^2 + \alpha\|x\|^2$$

2. *(Iterated Tikhonov regularization of order $l \in \mathbb{N}$)* For $\alpha > 0$ the approximate solution $x_\alpha^\delta = x_{\alpha,l}^\delta$ can be computed by the recursive formula

$$T^*Tx_{\alpha,i}^\delta + \alpha x_{\alpha,i}^\delta = T^*y^\delta + \alpha x_{\alpha,i-1}^\delta, \qquad i = 1, \ldots, N$$

and $x_{\alpha,0}^\delta = 0$. Since the same operator has to be inverted in all iteration steps, the computation of $x_{\alpha,i}^\delta$, $i \geq 2$, does not require much additional work.

3. *(Truncated Singular Value Decomposition, TSVD)* If T is compact, and $\{(\sigma_n, v_n, w_n) : n \in \mathbb{N}\}$ is a singular system for T then

$$x_\alpha^\delta = \sum_{n:\sigma_n \geq \alpha} \frac{1}{\sigma_n} \left\langle y^\delta, w_n \right\rangle v_n,$$

$\alpha > 0$. Usually, this method is only effective, if the singular values and functions of T are known explicitly since a numerical SVD is too expensive.

4. *(Landweber iteration)* Landweber iteration is defined by the recursion formula

$$x_k^\delta = x_{k-1}^\delta - T^*(y^\delta - Tx_{k-1}^\delta), \qquad k \in \mathbb{N} \tag{3.9}$$

and $x_0^\delta = 0$. We assume that $\|T\| \leq 1$. (Otherwise, we change the inner product in Y to $\omega \langle \cdot, \cdot \rangle$ with some scaling parameter $0 < \omega \leq \|T\|^{-2}$, and replace T^* by ωT^* in (3.9), correspondingly.) In order to treat Landweber iteration within the framework described above, we set $\alpha = (k+1)^{-1}$.

The following theorem implies that all these methods are regularization methods. Although this result is standard, we give a sketch of the proof since it is quite instructive and since parts of it are used later on.

Theorem 3.3. *Assume that the functions $g_\alpha, r_\alpha : \sigma(T^*T) \to \mathbb{R}$ are piecewise continuous and satisfy (3.6), (3.8), and*

$$|g_\alpha(\lambda)| \leq \frac{C_g}{\alpha}, \tag{3.10}$$

$$|r_\alpha(\lambda)| \leq C_r \tag{3.11}$$

for some constants $C_g, C_r > 0$ and all $\lambda \in \sigma(T^*T)$, $\alpha > 0$. Then the operators R_α defined by (3.5) together with the a-priori parameter choice strategy $\alpha(\delta) = \delta$ are regularization methods in the sense of Definition 3.1.

Proof. (3.10) implies that the operators R_α are bounded. By virtue of (3.6) and (3.7) we have

$$\|x^\dagger - x_\alpha\|^2 = \int_0^{\|T\|^2+} r_\alpha(\lambda)^2 \, \mathrm{d}\|E_\lambda x^\dagger\|^2 \tag{3.12}$$

with

$$\lim_{\alpha \searrow 0} r_\alpha(\lambda) = \begin{cases} 1, & \lambda = 0 \\ 0, & \lambda \in \sigma(T^*T)\backslash\{0\} \end{cases} . \tag{3.13}$$

Here $\{E_\lambda\}$ is the spectral family of T^*T, and we assume the convention that it is continuous from the left. In order to establish (3.3), we apply Lebesgue's dominated convergence theorem to the integral in (3.12) and use $x^\dagger \in N(T)^\perp$ and (3.11).

To prove (3.4) we split the total error into an *approximation error* and a *propagated data noise error*:

$$\|x^\dagger - x_\alpha^\delta\| \leq \|x^\dagger - x_\alpha\| + \|x_\alpha - x_\alpha^\delta\| \tag{3.14}$$

Using (3.10) and (3.11), it can be shown that

$$\|g_\alpha(T^*T)T^*\|^2 \leq \frac{C^2}{\alpha} \tag{3.15}$$

with $C = (C_g \cdot \sup_\lambda |\lambda g_\alpha(\lambda)|)^{1/2} \leq \sqrt{C_g(1 + C_r)}$. Therefore, the propagated data noise error can be estimated by

$$\|x_\alpha - x_\alpha^\delta\| \leq C \frac{\delta}{\sqrt{\alpha}} = C\sqrt{\delta}.$$

Now (3.4) follows from (3.3), (3.14), and (3.15). ■

Unfortunately, it can be shown that for ill-posed problems (in the sense that $T^\dagger$ is unbounded) the convergence (3.4) can be *arbitrarily slow* (cf., e.g., [EHN96, Proposition 3.11]). However, faster convergence and estimates on the convergence rates can be shown for certain $x^\dagger \in X$ that satisfy a so-called *source condition*. This means that there is some function $f \in C(\sigma(T^*T))$ with $f(0) = 0$ and a "source" $w \in X$ such that $x^\dagger$ has a representation

$$x^\dagger = f(T^*T)w, \qquad \|w\| \leq \rho. \tag{3.16}$$

As T is usually smoothing, (3.16) can be seen as an abstract smoothness condition. The behavior of f near 0 determines how much smoothness of $x^\dagger$ is required compared to the smoothing properties of T^*T. The faster f tends to 0, the more smoothness is implied by (3.16). The most commonly used choice is $f(\lambda) = \lambda^\mu$ with some $\mu > 0$, leading to a so-called *Hölder-type source condition*

$$x^\dagger = (T^*T)^\mu w, \qquad \|w\| \leq \rho. \tag{3.17}$$

Whereas conditions of the form (3.17) have natural interpretations for many mildly ill-posed problems, they are far too restrictive for most exponentially ill-posed problems. (3.17) often implies that $x^\dagger$ in an analytic function in such situations. As we will see, an appropriate choice of f for exponentially ill-posed problems is

$$f_p(\lambda) := \begin{cases} (-\ln \lambda)^{-p}, & 0 < \lambda \leq \exp(-1) \\ 0, & \lambda = 0 \end{cases} \tag{3.18}$$

with $p > 0$, i.e.

$$x^\dagger = f_p(T^*T)w, \qquad \|w\| \leq \rho. \tag{3.19a}$$

We call (3.19) a *logarithmic source condition.* In order to avoid the singularity of f_p at $\lambda = 1$, we always assume in this context that the norm in Y is scaled such that

$$\|T^*T\| = \|T\|^2 \leq \exp(-1). \tag{3.19b}$$

Of course, scaling the norm of Y has the same effect as scaling the operator T. The reason for choosing the value $\exp(-1)$ in (3.19) will become clear in Corollary 3.9.

In Section 3.7., we give some examples of important problems where (3.19) is equivalent to a smoothness condition in terms of Sobolev spaces.

3.2. Optimality

Assume we want to solve (3.1), we have noisy data satisfying (3.2) and the a-priori information that the exact solution satisfies a source condition, i.e. that $x^\dagger$ belongs to the *source set*

$$M_{f,\rho} := \{f(T^*T)w : w \in X \wedge \|w\| \leq \rho\}.$$

In this section we address the question: *What is the best possible general error estimate for any approximation to $x^\dagger$ that can be obtained from this* *information?* After answering this question, we define several degrees of optimality of regularization methods depending on how close the worst case error is to the best possible error estimate. Then, in the following sections, we determine the degree of optimality of commonly used regularization methods under logarithmic source conditions.

To rephrase the question above, let us assume that $R : Y \to X$ is an arbitrary mapping to approximately recover $x^\dagger$ from y^δ. We do not assume here that R is of the form of Definition 3.1 or that it is even continuous. Then the *worst case error for* R under the a-priori information $x^\dagger \in M_{f,\rho}$ is

$$\Delta_R(\delta, M_{f,\rho}, T) := \sup\{\|Ry^\delta - x^\dagger\| : x^\dagger \in M_{f,\rho} \wedge \|Tx^\dagger - y^\delta\| \leq \delta\}.$$

The *best possible error bound* is defined as the infimum over all mappings $R : Y \to X$:

$$\Delta(\delta, M_{f,\rho}, T) := \inf_R \Delta_R(\delta, M_{f,\rho}, T)$$

It turns out that the infimum is actually attained. The basic tool to construct such an optimal mapping is the "Melkman-Micchelli formula"

$$\begin{aligned} &\sup\{\|z\| : z \in Z, \|z\|_0 \leq 1, \|z\|_1 \leq 1\} \\ &\quad = \min_{0 \leq t \leq 1} \sup\{\|z\| : z \in Z, (1-t)\|z\|_0^2 + t\|z\|_1^2 \leq 1\} \end{aligned} \tag{3.20}$$

(cf. [MM80]), which holds for Hilbert-space semi-norms $\|\cdot\|$, $\|\cdot\|_0$, and $\|\cdot\|_1$ on a vector space Z. Moreover, Δ is equal to the modulus of continuity of T defined by

$$\omega(\delta, M_{f,\rho}, T) := \sup\{\|x\| : x \in M_{f,\rho} \wedge \|Tx\| \leq \delta\}.$$

Theorem 3.4. *The formula*

$$\Delta(\delta, M_{f,\rho}, T) = \Delta_{R^*}(\delta, M_{f,\rho}, T) = \omega(\delta, M_{f,\rho}, T)$$

holds. Here R^* *maps* $y^\delta \in Y$ *to the unique minimizer* x_α^δ *of the generalized Tikhonov functional*

$$\|Tx - y^\delta\|^2 + \alpha\|f(T^*T)^\dagger x\|^2$$

over $\operatorname{ran}(f(T^*T))$. *(The superscript* † *denotes the Moore-Penrose inverse.) The regularization parameter is* $\alpha = \frac{t}{1-t}\frac{\delta^2}{\rho^2}$ *where* t *is chosen according to (3.20) such that*

$$\begin{aligned} &\sup\{\|f(T^*T)w\| : w \in X, \rho^{-1}\|w\| \leq 1, \delta^{-1}\|Tf(T^*T)w\| \leq 1\} = \\ &\quad \sup\{\|f(T^*T)w\| : w \in X, t\rho^{-2}\|w\|^2 + (1-t)\delta^{-2}\|Tf(T^*T)w\|^2 \leq 1\}. \end{aligned}$$

Proof. The theorem is already contained in the paper by Melkman and Micchelli [MM80, Theorem 3.1]. A proof for $f(\lambda) = \lambda^\mu$, which has a straightforward generalization to other functions f, is given in [Lou89, Theorems 3.4.1, 4.2.7]. ■

An estimate on $\omega(\delta, M_{f,\rho}, T)$ has been given by Mair [Mai94] and Tautenhahn [Tau98]. We improve these results by computing the exact values of $w(\delta, M_{f,\rho}, T)$ instead of estimates that are sharp for certain values of δ/ρ accumulating at 0.

Lemma 3.5. (Jensen's inequality) *Assume that $\phi \in C([\alpha, \beta])$ with $\alpha, \beta \in \mathbb{R} \cup \{\pm\infty\}$ is convex, and let μ be a finite, positive Borel measure on some space E which will always be a finite interval in the following. Then*

$$\phi\left(\frac{\int \chi d\mu}{\int d\mu}\right) \leq \frac{\int \phi \circ \chi \, d\mu}{\int d\mu} \tag{3.21}$$

holds for all $\chi \in L^1(\mu)$ with $\alpha \leq \chi \leq \beta$ a.e. $d\mu$. (The right hand side may be infinite if $\alpha = -\infty$ or $\beta = \infty$.)

Proof. W.l.o.g. we may assume that $\int d\mu = 1$. Let $M := \int \chi d\mu$ and $s \in \mathbb{R}$ such that $\phi(M) + s(\xi - M) \leq \phi(\xi)$ for all $\xi \in [a, b]$. s exists because ϕ is convex, and $s = \phi'(M)$ if ϕ is differentiable at M. It follows that

$$\phi(M) + s(\chi - M) \leq \phi \circ \chi \qquad \text{a.e. } d\mu.$$

An integration $d\mu$ yields (3.21). ■

For the special case $\phi(t) = t^p$, $p > 1$, inequality (3.21) is

$$\int \chi d\mu \leq \left(\int \chi^p d\mu\right)^{\frac{1}{p}} \left(\int d\mu\right)^{\frac{1}{q}}$$

with $q = \frac{p}{p-1}$. From this form, we easily obtain Hölder's inequality

$$\int |a||b| d\bar{\mu} \leq \left(\int |a|^p d\bar{\mu}\right)^{\frac{1}{p}} \left(\int |b|^q d\bar{\mu}\right)^{\frac{1}{q}}$$

for positive Borel measures $\bar{\mu}$ on E, $a \in L^p(\bar{\mu})$, and $b \in L^q(\bar{\mu})$ by setting $\mu = |b|^q \bar{\mu}$ and $\chi = |a||b|^{-\frac{1}{p-1}}$.

Proposition 3.6. *Let (3.16) hold, and assume that* $f \in C([0,\tau])$, $\tau \geq \|T\|^2$, *is strictly monotonically increasing with* $f(0) = 0$. *Moreover, assume that the function* $\phi : [0, f(\tau)^2] \to [0, \tau f(\tau)^2]$ *defined by*

$$\phi(\xi) := \xi \cdot (f \cdot f)^{-1}(\xi) \tag{3.22}$$

is convex. Then the stability estimate

$$\|x\|^2 \leq \rho^2 \phi^{-1} \left(\frac{\|Tx\|^2}{\rho^2} \right). \tag{3.23}$$

holds. Consequently, for $\delta \leq \rho\sqrt{\tau} f(\tau)$,

$$\omega(\delta, M_{f,\rho}, T) \leq \rho \sqrt{\phi^{-1}\left(\delta^2/\rho^2\right)}. \tag{3.24}$$

Proof. By linearity, we may assume that $\rho = 1$. Let $\{E_\lambda\}$ be the spectral family of T^*T. Then (3.21) and (3.22) yield

$$\begin{aligned}
\phi\left(\frac{\|x\|^2}{\|w\|^2}\right) &= \phi\left(\frac{\int_0^\tau f(\lambda)^2 \,\mathrm{d}\|E_\lambda w\|^2}{\int_0^\tau \mathrm{d}\|E_\lambda w\|^2}\right) \\
&\leq \frac{\int_0^\tau \phi(f(\lambda)^2)\,\mathrm{d}\|E_\lambda w\|^2}{\int_0^\tau \mathrm{d}\|E_\lambda w\|^2} \\
&= \frac{\int_0^\tau \lambda f(\lambda)^2 \,\mathrm{d}\|E_\lambda w\|^2}{\|w\|^2} \\
&= \frac{\|Tx\|^2}{\|w\|^2}.
\end{aligned}$$

By the convexity of ϕ, the fact that $\phi(0) = 0$, and $\|w\| \leq 1$, this estimate implies

$$\phi(\|x\|^2) \leq \|Tx\|^2. \tag{3.25}$$

Since f is strictly increasing, so are $f \cdot f$, $(f \cdot f)^{-1}$, ϕ, and ϕ^{-1}. Hence, applying ϕ^{-1} to (3.25) yields (3.23). (3.24) follows from (3.23) and the definition. ■

Remark 3.7. If x is an eigenvector of T^*T, i.e. $T^*Tx = \lambda x$, then equality holds in (3.23). Since $x = f(\lambda)w$ and

$$\|Tx\|^2 = \|(T^*T)^{1/2}x\|^2 = \|\sqrt{\lambda} f(\lambda) w\|^2,$$

we have to show that

$$f(\lambda)^2 = \phi^{-1}(\lambda f(\lambda)^2).$$

After substituting $\xi = f(\lambda)^2$ and applying ϕ, this is (3.22). This straightforward calculation may serve as a motivation for the definition (3.22) of ϕ. Moreover, we see that equality holds in (3.24) if $(\delta/\rho)^2$ is an eigenvalue of $T^*Tf(T^*T)^2$.

For the usual choice $f(\lambda) = \lambda^\mu$, $\mu > 0$, we have $\phi(\xi) = \xi^{\frac{1+2\mu}{2\mu}}$. Obviously, the assumptions of Proposition 3.6 are satisfied, and we obtain the following classical result, which is usually proved by interpolation. Proposition 3.6 may often serve as a substitute for interpolation when working with general sources conditions.

Corollary 3.8. *(3.17) implies*

$$\|x\| \le \rho^{\frac{1}{1+2\mu}} \|Tx\|^{\frac{2\mu}{1+2\mu}}.$$

Moreover,

$$\omega(\delta, M_{\lambda^\mu,\rho}, T) \le \rho^{\frac{1}{2\mu+1}} \delta^{\frac{2\mu}{1+2\mu}}.$$

The case $f = f_p$ (cf. (3.18)) has been considered by Mair [Mai94].

Corollary 3.9. *The assumptions of Proposition 3.6 are satisfied for $f = f_p$, and the inverses of the corresponding functions ϕ_p have the asymptotic behavior*

$$\sqrt{\phi^{-1}(\lambda)} = f_p(\lambda)(1 + o(1)), \qquad \lambda \to 0. \tag{3.26}$$

Consequently,

$$\|x\| \le \rho f_p\left(\frac{\|Tx\|^2}{\rho^2}\right)(1 + o(1)) \tag{3.27}$$

$$\omega(\delta, M_{f_p,\rho}, T) \le \rho f_p\left(\delta^2/\rho^2\right)(1 + o(1)). \tag{3.28}$$

Proof. By (3.19b), we have $\tau = \exp(-1)$. It is obvious that f_p is continuous on $[0, \tau]$ and strictly monotonically increasing. $\phi : [0, 1] \to [0, \exp(-1)]$ is given by

$$\phi(\xi) = \xi \exp(-\xi^{-\frac{1}{2p}}).$$

From

$$\phi''(\xi) = \exp(-\xi^{-1/2p}) \frac{\xi^{-1-\frac{1}{2p}}}{(2p)^2}(2p - 1 + \xi^{-\frac{1}{2p}})$$

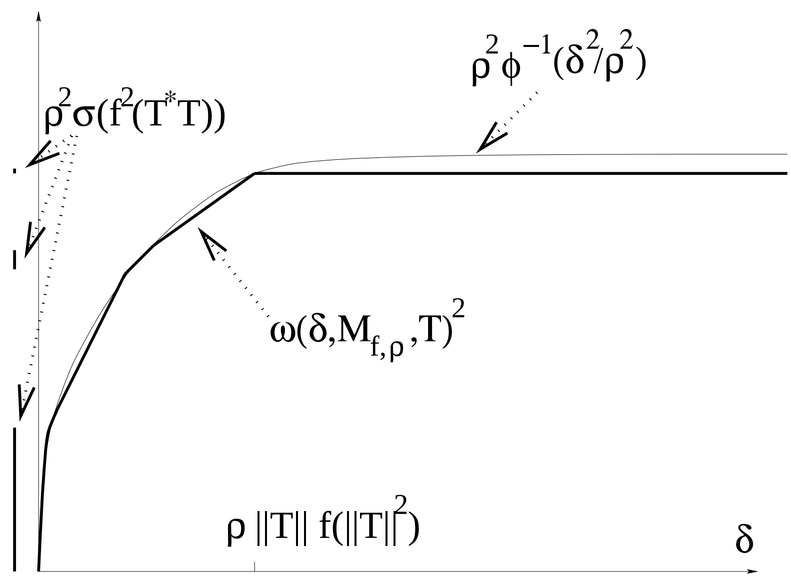


Figure 3.1: Illustration of Theorem 3.10

it is easily seen that $\phi''(\xi) \geq 0$ for $\xi \in [0, 1]$, i.e. ϕ is is convex.

To prove the estimate on $\sqrt{\phi^{-1}(\lambda)}$, first note that $\xi = \phi^{-1}(\lambda)$ implies

$$\ln \lambda = \ln \xi - \xi^{-\frac{1}{2p}}.$$

Therefore,

$$\begin{aligned} \xi &= (\ln \xi - \ln \lambda)^{-2p} \\ &= (-\ln \lambda)^{-2p} \left(1 - \frac{\ln \xi}{\ln \lambda}\right)^{-2p} \\ &= f_p(\lambda)^2 \left(1 - \frac{\ln \xi}{\ln \xi - \xi^{-\frac{1}{2p}}}\right)^{-2p} \end{aligned}$$

Since $\lim_{\xi\to 0} \frac{\ln \xi}{\ln \xi - \xi^{-1/2p}} = 0$ and $\lim_{\lambda\to 0} \xi = \lim_{\lambda \to 0} \phi^{-1}(\lambda) = 0$, the assertion follows. ■

Now, we compute the exact values of the modulus of continuity.

Theorem 3.10. *Let the assumptions of Proposition 3.6 hold. Define the function* $\tilde{\phi} : [0, f(\tau)^2] \to [0, \tau f(\tau)^2]$ *by*

$$\tilde{\phi}(\xi) := \begin{cases} \phi(\xi), & \xi \in \sigma(f^2(T^*T)) \\ \frac{\xi_+ - \xi}{\xi_+ - \xi_-}\phi(\xi_-) + \frac{\xi - \xi_-}{\xi_+ - \xi_-}\phi(\xi_+), & \textit{else} \end{cases}$$

where

$$\begin{aligned}\xi_- &:= \sup\{\tilde{\xi} \in \sigma(f^2(T^*T)) : \tilde{\xi} \le \xi\},\\ \xi_+ &:= \inf\{\tilde{\xi} \in \sigma(f^2(T^*T)) : \tilde{\xi} \ge \xi\}.\end{aligned}$$

Then

$$\omega(\delta, M_{f,\rho}, T) = \rho\sqrt{\tilde{\phi}^{-1}(\delta^2/\rho^2)} \tag{3.29}$$

for $\delta \le \rho\|T\| f(\|T\|^2)$, *and* $\omega(\delta, M_{f,\rho}, T) = \rho f(\|T\|^2)$ *for* $\delta > \rho\|T\|f(\|T\|^2)$.

Proof. If $\delta > \rho\|T\|f(\|T\|^2)$, then $\|Tx\| \le \delta$ holds for all $x \in M_{f,\rho}$, so we have $\omega(\delta, M_{f,\rho}, T) = \sup\{\|x\| : x \in M_{f,\rho}\}$.

Let us now prove (3.29). Since $\tilde{\phi}$ is convex, increasing, $\tilde{\phi}(0) = 0$, and $\tilde{\phi} = \phi$ on $\sigma(f^2(T^*T))$ (note that $\tilde{\phi}$ is the greatest function with these properties!), the proof of Proposition 3.6 is also valid with ϕ replaced by $\tilde{\phi}$. This yields "$\le$" in (3.29).

It remains to prove "$\ge$" in (3.29). We assume that δ^2/ρ^2 is not in $\sigma(T^*Tf(T^*T)^2)$. For $\delta^2/\rho^2 \in \sigma(T^*Tf(T^*T)^2)$, the proof is similar to the one below, but simpler. The special case that δ^2/ρ^2 is an eigenvalue has been treated in Remark 3.7. The idea of this part of the proof is to construct a sequence $\{x_n\} \subset M_{f,\rho}$ with $\|Tx_n\| \le \delta$ such that $\lim_{n\to\infty} \|x_n\|^2 = \rho^2\tilde{\phi}^{-1}(\delta^2/\rho^2)$.

Define $\xi := \tilde{\phi}^{-1}(\delta^2/\rho^2)$, $\xi_\pm$ as in the theorem, and $\lambda, \lambda_+, \lambda_-$ by $\xi = f(\lambda)^2$ and $\xi_\pm = f(\lambda_\pm)^2$. Equivalently, $\lambda_+ = \inf\{\tilde{\lambda} \in \sigma(T^*T) : \tilde{\lambda} \ge \lambda\}$ since $f^2(\sigma(T^*T)) = \sigma(f^2(T^*T))$ by the spectral mapping theorem. Hence, $\lambda_+ \in \sigma(T^*T)$ due to the closedness of the spectrum. Analogously, we have $\lambda_- \in \sigma(T^*T)$. Therefore, denoting the spectral family of T^*T by $\{E_\lambda\}$, we can choose $\omega_n^+ \in \operatorname{ran}(E_{\lambda_+ + \frac{1}{n}} - E_{\lambda_+})$ and $\omega_n^- \in \operatorname{ran}(E_{\lambda_-} - E_{\lambda_- - \frac{1}{n}})$ with $\|\omega_n^+\| = \|\omega_n^-\| = \rho$ for all $n \in \mathbb{N}$. Define $x_n^\pm := f(T^*T)\omega_n^\pm$. From $\|Tx_n^\pm\|^2 = \int \tilde{\lambda} f(\tilde{\lambda})^2 \,\mathrm{d}\|E_{\tilde{\lambda}} w_n^\pm\|^2$ we find

$$\begin{aligned}\lambda_+ f(\lambda_+)^2\rho^2 \le \quad \|Tx_n^+\|^2 &\le \left(\lambda_+ + \frac{1}{n}\right) f\left(\lambda_+ + \frac{1}{n}\right)^2 \rho^2,\\ \left(\lambda_- - \frac{1}{n}\right) f\left(\lambda_- - \frac{1}{n}\right)^2 \rho^2 \le \quad \|Tx_n^-\|^2 &\le \lambda_- f(\lambda_-)^2\rho^2.\end{aligned}$$

This implies $\|Tx_n^\pm\|^2 \to \lambda_\pm f(\lambda_\pm)^2\rho^2$ as $n \to \infty$, and analogously, it can be shown that $\|x_n^\pm\|^2 \to f(\lambda_\pm)^2\rho^2 = \xi_\pm\rho^2$. Since

$$\operatorname{ran}(E_{\lambda_-} - E_{\lambda_- - \frac{1}{n}}) \perp \operatorname{ran}(E_{\lambda_+ + \frac{1}{n}} - E_{\lambda_+}),$$

we have $\langle \omega_n^-, \omega_n^+ \rangle = \langle x_n^-, x_n^+ \rangle = \langle Tx_n^-, Tx_n^+ \rangle = 0$ for all n. Define $\alpha := \left(\frac{\xi_+ - \xi}{\xi_+ - \xi_-}\right)^{1/2}$ and $\beta := \left(\frac{\xi - \xi_-}{\xi_+ - \xi_-}\right)^{1/2}$. Then, with $\delta_n := \|\alpha T x_n^- + \beta T x_n^+\|$, we have

$$\begin{aligned}
\delta_n^2 &= \alpha^2 \|Tx_n^-\|^2 + \beta^2 \|Tx_n^+\|^2 \\
&\overset{n\to\infty}{\to} \left(\alpha^2 \lambda_- f(\lambda_-)^2 + \beta^2 \lambda_+ f(\lambda_+)^2\right) \rho^2 \\
&= \left(\alpha^2 \phi(\xi_-) + \beta^2 \phi(\xi_+)\right) \rho^2 \\
&= \tilde{\phi}(\xi) \rho^2 = \delta^2.
\end{aligned}$$

We now set $\omega_n := \min(1, \delta/\delta_n)(\alpha \omega_n^- + \beta \omega_n^+)$, and $x_n := f(T^*T)\omega_n$. Note that $x_n \in M_{f,\rho}$ as $\|\omega_n\| = \min(1, \delta/\delta_n)\rho \leq \rho$, and that $\|Tx_n\| = \min(1, \delta/\delta_n)\delta_n \leq \delta$. Hence,

$$\begin{aligned}
\omega(\delta, \rho, T)^2 &\geq \sup_{n \in \mathbb{N}} \|x_n\|^2 \geq \lim_{n\to\infty} (\min(1, \delta/\delta_n))^2 (\alpha^2 \|x_n^-\|^2 + \beta^2 \|x_n^+\|^2) \\
&= \rho^2 \left(\alpha^2 f(\lambda_-)^2 + \beta^2 f(\lambda_+)^2\right) \\
&= \rho^2 (\alpha^2 \xi_- + \beta^2 \xi_+) \\
&= \rho^2 \xi = \rho^2 \tilde{\phi}^{-1}(\delta^2/\rho^2).
\end{aligned}$$

■

This theorem has obvious implications for the source conditions (3.17) and (3.19) that we do not state explicitly. It completes the answer to the question raised at the beginning of this section. We end this section with a discussion of optimality of regularization methods.

Definition 3.11. Let R_α be a regularization method for (3.1) with parameter choice rule $\alpha = \alpha(\delta, y^\delta)$, and let the assumptions of Proposition 3.6 be satisfied. Convergence on the source sets $M_{f,\rho}$ is said to be

- *optimal* if
$$\Delta_{R_\alpha}(\delta, M_{f,\rho}, T) \leq \rho \sqrt{\phi^{-1}(\delta^2/\rho^2)}$$

- *asymptotically optimal* if
$$\Delta_{R_\alpha}(\delta, M_{f,\rho}, T) = \rho \sqrt{\phi^{-1}(\delta^2/\rho^2)}\, (1 + \mathrm{o}(1)), \qquad \delta \to 0$$

- *of optimal order* if there is a constant $C \geq 1$ such that
$$\Delta_{R_\alpha}(\delta, M_{f,\rho}, T) \leq C \rho \sqrt{\phi^{-1}(\delta^2/\rho^2)}$$
for δ/ρ sufficiently small.

Obviously, optimality implies asymptotic optimality, and asymptotic optimality implies order optimality.

Note that we have followed the convention to define optimality over the estimate $\rho\sqrt{\phi^{-1}(\delta^2/\rho^2)}$ on $\Delta(\delta, M_{f,\rho}, T)$ given in (3.24), although there exists a method described in Theorem 3.4 that is optimal in the strict sense that $\Delta_{R^*} = \Delta$. The term "optimal" is justified in the sense that $\rho\sqrt{\phi^{-1}(\delta^2/\rho^2)}$ is the best-possible estimate on $\Delta(\delta, M_{f,\rho}, T)$ *independent of* T. Another reason for this choice of terminology is that the parameter choice rule needed in the method R^* in Theorem 3.4 is very hard to implement in general. On the other hand, Vainikko [Vai86] has constructed parameter choice rules for a class of regularization methods that are much easier to implement and lead to optimal convergence in the sense of Definition 3.11 (cf. also [Lou89]). A similar analysis for more general source conditions has been given by Tautenhahn [Tau98]. The concept of asymptotic optimality has been introduced as a substitute for optimality for iterative methods.

However, all these methods require exact knowledge of a source set $M_{f,\rho}$ that contains the solution. In the simplest cases this may correspond to knowing the exact smoothness of the true solution and its size in a corresponding Sobolev-norm. Such information is usually not available in practice. Therefore, a lot of work has been done to develop a-posteriori parameter choice rules that yield at least order-optimal convergence for Hölder-type source conditions and do not require knowledge of the smoothness parameter μ in (3.17) (see [EHN96] and the references therein).

In Section 3.3. we will see that the simple a-priori parameter choice rule $\alpha \sim \delta$ leads to order-optimal convergence rates on the logarithmic source sets $M_{f_p,\rho}$ for all $p, \rho > 0$. In Section 3.5. we prove that even asymptotically optimal convergence rates can be obtained without knowledge of the parameters p and ρ in (3.19).

3.3. A-priori parameter choice rules

We start with the following simple estimates of the approximation error and its image under T which is indispensable for the analysis in the following sections.

Proposition 3.12. *Assume that $x^\dagger$ satisfies (3.19). If*

$$f_p(\lambda)|r_\alpha(\lambda)| \le C_1 f_p(\alpha) \tag{3.30}$$

holds for $\alpha, \lambda \in [0, \exp(-1)]$ with a constant C_1 depending only on p, then

$$\|x_\alpha - x^\dagger\| \le C_1 f_p(\alpha)\rho. \tag{3.31}$$

If

$$\sqrt{\lambda} f_p(\lambda)|r_\alpha(\lambda)| \le C_2 \sqrt{\alpha} f_p(\alpha) \tag{3.32}$$

with C_2 *depending only on* p, *then*

$$\|Tx_\alpha - Tx^\dagger\| \le C_2 \sqrt{\alpha} f_p(\alpha)\rho. \tag{3.33}$$

Proof. (3.31) follows from $x_\alpha - x^\dagger = r_\alpha(T^*T)f_p(T^*T)w$ and the isometry of the functional calculus. The proof of (3.33) is analogous and uses the identity $\|Tz\| = \|(T^*T)^{1/2}z\|$ which holds for all $z \in X$. ∎

For Hölder-type source conditions, the condition corresponding to (3.30) and (3.32) is

$$\lambda^\mu |r_\alpha(\lambda)| \le C_3 \alpha^\mu. \tag{3.34}$$

In the next lemma we show that (3.34) implies (3.30) and (3.32). Therefore, Proposition 3.12 applies to most commonly used regularization methods. This generalizes and simplifies corresponding results in [Hoh97] for Tikhonov regularization and in [DES98] for Landweber iteration.

Lemma 3.13.

1. *(3.34) for any* $\mu > 0$ *and (3.11) imply (3.30) for all* $p > 0$.
2. *(3.34) for any* $\mu > 1/2$ *and (3.11) imply (3.32) for all* $p > 0$.
3. *For all regularization methods in Example 3.2, (3.34) and (3.11) are satisfied for* $\mu \le 1$. *Hence (3.30) and (3.32) hold for all* $p > 0$.

Proof. We make the substitution $q = \alpha/\lambda$ and write $\tilde{r}(\lambda, q) := r_{q\lambda}(\lambda)$ with $q \in [0, 1/(\mathrm{e}\lambda)]$. Then (3.30), (3.32), and (3.34) transform to

$$\tilde{r}(\lambda, q) \le C_1 \frac{f_p(q\lambda)}{f_p(\lambda)}, \tag{3.35}$$

$$\tilde{r}(\lambda, q) \le C_2 \sqrt{q} \frac{f_p(q\lambda)}{f_p(\lambda)}, \tag{3.36}$$

$$\tilde{r}(\lambda, q) \le C_3 q^\mu, \tag{3.37}$$

rsp. Suppose, that (3.37) and (3.11) hold for some $\mu > 0$. Then there exists a constant $C > 0$ depending on p such that for $0 < q \le 1$ and $0 < \lambda \le 1/\mathrm{e}$ the estimate

$$\begin{aligned} \tilde{r}(\lambda, q) &\le C_3 q^\mu \le C(-\ln q + 1)^{-p} \\ &\le C\left(\frac{\ln q}{\ln \lambda} + 1\right)^{-p} = C \frac{f_p(q\lambda)}{f_p(\lambda)} \end{aligned}$$

holds. For $1 < q \le 1/(e\lambda)$, (3.11) implies that

$$\frac{f_p(q\lambda)}{f_p(\lambda)} > 1 \ge \frac{\tilde{r}(\lambda, q)}{C_r}.$$

This proves the first assertion, and the second is shown analogously.

	Tikhonov	iter. Tikhonov	TSVD	Landweber
$\tilde{r}(\lambda, q)$:	$\frac{q}{q+1}$	$\left(\frac{q}{q+1}\right)^l$	$0, \; q \le 1$ $1, \; q > 1$	$(1-\lambda)^{1/(\lambda q)}$

It is easily seen that the functions $\tilde{r}$ listed in the table above satisfy (3.37), and hence (3.34). (For Landweber iteration, this follows from $(1-\lambda)^{1/\lambda} \le 1/e$; we have set $q = 1/(k\lambda)$.) This proves the last assertion and finishes the proof. ∎

We now obtain the main result of this section.

Theorem 3.14. *Assume that (3.10), (3.11), and (3.30) hold, and that $x^\dagger$ satisfies a source condition (3.19) for some $p > 0$. Then the regularized solutions $R_\alpha y^\delta$ with $\alpha(\delta) = \gamma\frac{\delta}{\rho}$, $\gamma > 0$, and R_α given by (3.5) satisfy the order-optimal estimate*

$$\|x^\dagger - x_\alpha^\delta\| \le C\rho f_p(\delta^2/\rho^2)$$

for δ/ρ sufficiently small with a constant C depending on p, γ, and the regularization method.

Proof. If $\gamma\delta/\rho \le \exp(-1)$ and $\delta/\rho \le \gamma^{-2}$, we have

$$\begin{aligned}\|x^\dagger - x_\alpha^\delta\| &\le \|x^\dagger - x_\alpha\| + \|x_\alpha - x_\alpha^\delta\| \le C_1\rho f_p(\alpha) + C\frac{\delta}{\sqrt{\alpha}} \\ &\le C_1\rho f_p\left(\gamma\frac{\delta}{\rho}\right) + C\rho\sqrt{\frac{\delta}{\gamma\rho}} \le C\rho f_p\left(\frac{\delta^2}{\rho^2}\right).\end{aligned}$$

with a generic constant C since $f_p(\gamma\delta/\rho) = 2^p\left(-\ln\delta^2/\rho^2 + \ln\gamma^{-2}\right)^{-p} \le 2^{2p} f_p(\delta^2/\rho^2)$. ∎

Note that order-optimal convergence also holds for the choice $\alpha = \delta$, but with a constant depending on ρ. For Tikhonov regularization this has been observed by Mair [Mai94]. This result is remarkable as for Hölder-type source conditions (3.17) it is not possible to obtain order-optimal convergence rates by an a-priori parameter choice rule without knowledge of the smoothness parameter μ.

3.4. A converse result

The following theorem states that the source condition (3.19) is not only sufficient for the rate (3.31) in Proposition 3.12, but also *almost* necessary.

Theorem 3.15. *Assume that (3.6), (3.10), and (3.11) hold. Then the estimate*

$$\|x^\dagger - x_\alpha\| = \mathrm{O}\left(f_q(\alpha)\right), \qquad \alpha \searrow 0 \tag{3.38}$$

for some $q > 0$ *implies that (3.19) holds for all* $0 < p < q$.

Proof. The proof is modeled after the proofs of Lemma 4.12. and Proposition 4.13. in [EHN96]. We use (3.10) to obtain the lower bound

$$|r_\alpha(\lambda)| \geq 1 - \lambda |g_\alpha(\lambda)| \geq 1 - \frac{C_g \lambda}{\alpha} \geq \frac{1}{2}$$

for $\lambda \in [0, \frac{\alpha}{2C_g}]$. Then, by (3.12), we have

$$\begin{aligned} \|x^\dagger - x_\alpha\|^2 &\geq \int_0^{\alpha/2C_g} |r_\alpha(\lambda)|^2 \, \mathrm{d}\|E_\lambda x^\dagger\|^2 \\ &\geq \frac{1}{4} \int_0^{\alpha/2C_g} \mathrm{d}\|E_\lambda x^\dagger\|^2 = \frac{1}{4} \|E_{\alpha/2C_g} x^\dagger\|^2, \end{aligned}$$

and (3.38) implies

$$\|E_\epsilon x^\dagger\| = \mathrm{O}\left(f_q(2C_g\epsilon)\right) = \mathrm{O}\left(f_q(\epsilon)\right), \qquad \epsilon \searrow 0. \tag{3.39}$$

This and a partial integration yield

$$\begin{aligned} \int_\epsilon^{\|T\|^2+} f_p(\lambda)^{-2} \, \mathrm{d}\|E_\lambda x^\dagger\|^2 &= f_p(\|T\|^2)^{-2} \|x^\dagger\|^2 - f_p(\epsilon)^{-2} \|E_\epsilon x^\dagger\|^2 \\ &\quad + \int_\epsilon^{\|T\|^2+} \frac{2p}{\lambda} (-\ln \lambda)^{2p-1} \|E_\lambda x^\dagger\|^2 \, \mathrm{d}\lambda \\ &\leq C(1 + \int_\epsilon^{\|T\|^2+} \frac{2p}{\lambda} (-\ln \lambda)^{2p-1-2q} \, \mathrm{d}\lambda) \\ &= C(1 + \frac{p}{p-q} (-\ln \lambda)^{2p-2q}) \Big|_{\lambda=\epsilon}^{\lambda=\|T\|^2} . \end{aligned}$$

for some constant $C > 0$. As $p < q$, we have

$$\int_0^{\|T\|^2+} f_p(\lambda)^{-2} \, \mathrm{d}\|E_\lambda x^\dagger\|^2 < \infty,$$

and this implies (3.19). ∎

3.5. An a-posteriori rule leading to asymptotically optimal convergence

Even though we have seen in Section 3.3. that the simple a-priori parameter choice rule $\alpha = \delta$ leads to order-optimal convergence rates under logarithmic source conditions, we recommend to use an a-posteriori stopping rule as described in this section which leads to asymptotically optimal error estimates for most regularization methods. Since convergence for logarithmic source conditions is so slow, it is important to have at least constants of reasonable size in the asymptotic behavior of the error. This is illustrated by the fact that in order to reduce the error in the approximate solution for $p = \rho = 1$ by a factor 10, the noise level δ in the data has to be replaced by δ^{10}! Note that the constant C_1 in the estimates in Section 3.3. deteriorates for large p.

We suggest to chose $\alpha = \alpha(\delta, y^\delta)$ such that the following conditions are satisfied:

$$\|Tx_\alpha^\delta - y^\delta\| \leq 2\delta \max(-\ln\delta, 1) \tag{3.40a}$$

$$\alpha \leq \exp(-1) \tag{3.40b}$$

$$\alpha < \exp(-1) \;\Rightarrow\; \exists \alpha' \in [\alpha, 2\alpha]\; \|Tx_{\alpha'}^\delta - y^\delta\| \geq 2\delta\max(-\ln\delta, 1) \tag{3.40c}$$

An alternative to (3.40c) is

$$\alpha < \exp(-1) \;\Rightarrow\; \|Tx_\alpha^\delta - y^\delta\| \geq \frac{3}{2}\delta\max(-\ln\delta, 1) \tag{3.40d}$$

Obviously, these parameter choice rules are related to the well-known *discrepancy principle.*

The next lemma shows that for most regularization methods a parameter α satisfying (3.40a)-(3.40c) exists and can be found by a simple algorithm.

Lemma 3.16. *Assume that (3.2), (3.6), and (3.11) with* $C_r = 1$ *hold and that* $\delta > 0$*. If* (α_n) *is some sequence of positive numbers converging monotonically decreasing to* 0 *with* $\alpha_0 = \exp(-1)$ *and* $\alpha_n/\alpha_{n+1} \leq 2$*, then the algorithm*

$$\begin{aligned}
&n := 0\\
&\text{while } \|Tx_{\alpha_n}^\delta - y^\delta\| > 2\delta\max(-\ln\delta, 1)\\
&\qquad n := n+1
\end{aligned}$$

terminates after a finite number N *of steps and yields a number* $\alpha = \alpha_N$ *satisfying (3.40a)-(3.40c) with* $\alpha' = \alpha_{N-1}$ *if* $N > 0$.

Proof. Obviously, it suffices to prove that

$$\lim_{\alpha\to 0} \|Tx_\alpha^\delta - y^\delta\| < 2\delta.$$

Note that the identity

$$y^\delta - Tx_\beta^\delta = (I - Tg_\beta(T^*T)T^*)y^\delta = r_\beta(TT^*)y^\delta \tag{3.41}$$

holds for all $\beta > 0$ since $g_\beta(T^*T)T^* = T^*g_\beta(TT^*)$ (cf. [EHN96, eq. (2.43)]).

As in the proof of Theorem 3.3, Lebesgue's dominated convergence theorem and (3.13) yield

$$\lim_{\alpha\to\infty} \|Tx_\alpha^\delta - y^\delta\|^2 = \|P_{N(T^*)}y^\delta\|^2$$

where $P_{N(T^*)}$ is the orthogonal projection on $N(T^*) = \mathrm{ran}(T)^\perp$. Since $y \in \mathrm{ran}(T)$, we have

$$\|P_{N(T^*)}y^\delta\| = \|P_{N(T^*)}(y^\delta - y)\| \leq \delta.$$

This completes the proof. ■

For iterative methods, a natural choice of α_n is $\alpha_n = \exp(-1)/(n+1)$ where n is the iteration number. In case of continuous regularization, a parameter α satisfying (3.40a)-(3.40c) can be found by a simple bisection algorithm, i.e $\alpha_n = \exp(-1)\cdot 2^{-n}$. For Tikhonov regularization faster convergence is achieved by a Newton method applied to the function $1/\alpha \mapsto \|Tx_\alpha^\delta - y^\delta\|$ (cf. [EHN96, Proposition 9.8]). Here (3.40d) is more appropriate.

Theorem 3.17. *Assume that the functions r_α and g_α satisfy (3.6), (3.10), (3.11) with $C_r = 1$, and (3.32), that $\alpha = \alpha(\delta, y^\delta)$ is chosen such that (3.40a), (3.40b), and either (3.40c) or (3.40d) hold, and that $x^\dagger$ satisfies a logarithmic source condition (3.19). Then the asymptotically optimal estimate*

$$\|x_\alpha^\delta - x^\dagger\| \leq \rho f_p(\delta^2/\rho^2)(1 + \mathrm{o}\,(1))$$

holds for $\delta \to 0$.

Proof. W.l.o.g we may assume that $\delta \leq \exp(-1)$. Then $\max(-\ln\delta, 1) = -\ln\delta$. We treat the approximation error $\|x^\dagger - x_\alpha\|$ and the propagated data noise error $\|x_\alpha - x_\alpha^\delta\|$ separately.

1.) To get an estimate on the *approximation error*, we apply Proposition 3.6 to $r_\alpha(T^*T)x^\dagger = f_p(T^*T)r_\alpha(T^*T)w$ and obtain

$$\|x^\dagger - x_\alpha\| \leq \rho\sqrt{\phi_p^{-1}\left(\frac{\|y - Tx_\alpha\|^2}{\rho^2}\right)} \tag{3.42}$$

since $\|r_\alpha(T^*T)w\| \le C_r\|w\| \le \rho$. (3.40a) and the estimate

$$\|(y - Tx_\alpha) - (y^\delta - Tx_\alpha^\delta)\| = \|r_\alpha(TT^*)(y - y^\delta)\| \le \delta, \tag{3.43}$$

which follows from (3.2), (3.41), and $\|r_\alpha(TT^*)\| = C_r = 1$, imply

$$\|y - Tx_\alpha\| \le (1 - 2\ln\delta)\delta. \tag{3.44}$$

Plugging this into (3.42) and using (3.26) we obtain the upper bound

$$\begin{aligned} \|x^\dagger - x_\alpha\| &\le \rho\sqrt{\phi_p^{-1}\left(\frac{(1-2\ln\delta)^2\delta^2}{\rho^2}\right)} \\ &= \rho f_p\left((1-\ln\delta^2)^2\frac{\delta^2}{\rho^2}\right)(1 + \mathrm{o}(1)). \end{aligned}$$

Since

$$\begin{aligned} f_p\left((1-\ln\delta^2)^2\frac{\delta^2}{\rho^2}\right) &= f_p(\delta^2/\rho^2)\left(1 + \frac{-\ln(1-\ln\delta^2)^2}{-\ln\delta^2/\rho^2}\right)^{-p} \\ &= f_p(\delta^2/\rho^2)(1 + \mathrm{o}(1)), \end{aligned}$$

we have

$$\|x^\dagger - x_\alpha\| \le \rho f_p(\delta^2/\rho^2)(1 + \mathrm{o}(1)).$$

2.) To estimate the *propagated data noise error*, let us first assume that $\alpha < \exp(-1)$. Then, by (3.40c) and (3.43),

$$\|Tx_{\alpha'} - y\| \ge \|Tx_{\alpha'}^\delta - y^\delta\| - \delta \ge \delta(-\ln\delta)$$

holds. This together with (3.33) yields

$$\delta(-\ln\delta) \le \|Tx_{\alpha'} - y\| \le C_2\rho\sqrt{\alpha'}f_p(\alpha') \le C_2\rho\chi_p(\sqrt{\alpha'}) \tag{3.45}$$

where $\chi_p(\lambda) := \lambda\, f_p(\lambda)$. Obviously, (3.45) also holds for $\alpha = \exp(-1)$ if δ is sufficiently small. (3.15), (3.45), and the monotonicity of χ_p imply

$$\|x_\alpha - x_\alpha^\delta\| \le C\frac{\delta}{\sqrt{\alpha}} \le \sqrt{2}C\frac{\delta}{\sqrt{\alpha'}} \le \sqrt{2}C\frac{\delta}{\chi_p^{-1}(\delta(-\ln\delta)/(C_2\rho))}$$

where C is a generic constant. A very similar calculation gives the same result with (3.40d) instead of (3.40c). With the asymptotic formula for χ_p^{-1} shown in the following lemma and a computation similar to (3.5.) we obtain

$$\|x_\alpha - x_\alpha^\delta\| = C\rho(-\ln\delta)^{-1}\left(-\ln\frac{\delta(-\ln\delta)}{C_2\rho}\right)^{-p}(1 + \mathrm{o}(1)) = \rho f_p(\delta^2/\rho^2)\,\mathrm{o}(1)\,.$$

Combining this with the result of the first part of the proof gives the assertion.

■

The proof of the next lemma uses the same technique as the proof of Corollary 3.9 (see also [Tau98]).

Lemma 3.18. *The inverse of the function* $\chi_p(\lambda) := \lambda(-\ln\lambda)^{-p}$ *has the asymptotic behavior*

$$\chi_p^{-1}(\xi) = \xi(-\ln\xi)^p(1 + \mathrm{o}\,(1)), \qquad \xi \to 0.$$

Proof. Note that χ_p is strictly monotonically increasing and that $\chi_p(\lambda) \to 0$ as $\lambda \nearrow 0$, so χ_p^{-1} exists, and $\lim_{\xi\nearrow 0}\chi_p^{-1}(\xi) = 0$. If $\lambda = \chi_p^{-1}(\xi)$, then

$$\begin{aligned}
\chi_p^{-1}(\xi) &= \xi(-\ln\xi)^p \frac{\lambda}{\xi(-\ln\xi)^p} \\
&= \xi(-\ln\xi)^p \frac{\lambda}{\chi_p(\lambda)(-\ln\chi_p(\lambda))^p} \\
&= \xi(-\ln\xi)^p \left(\frac{-\ln\chi_p(\lambda)}{-\ln\lambda}\right)^{-p} \\
&= \xi(-\ln\xi)^p \left(1 + p\frac{\ln(-\ln\lambda)}{-\ln\lambda}\right)^{-p}.
\end{aligned}$$

Since $\lim_{t\to\infty} t^{-1}\ln t = 0$, this implies the assertion. ∎

If $2\delta\max(-\ln\delta, 1)$ in (3.40a) and (3.40c) is replaced by $\tau\delta$ with some constant $\tau > C_r \geq 1$, then at least order-optimal convergence can be shown.

3.6. Operator approximations

In this section we consider the situation that we want to solve an operator equation

$$F(x) = y, \qquad y \in \mathrm{ran}(F)$$

with an injective, not necessarily linear operator $F : X \supset D(F) \to Y$ that is given only approximately by a linear operator $T_h \in L(X, Y)$, $h > 0$ such that

$$\|F(x) - T_h x\| \leq h\|x\| \tag{3.46}$$

holds for all $x \in X$. Let $x^\dagger \in D(F)$ be the exact solution, $y := F(x^\dagger)$ the exact data and $y^\delta \in Y$ the measurement data satisfying (3.2). Moreover, we assume that there exists a linear operator $T \in L(X,Y)$, e.g. $T = F'[x^\dagger]$ such that

$$\|T - T_h\| \le h \tag{3.47}$$

and that $x^\dagger$ satisfies a logarithmic source condition (3.19) with T.

The error in the operator T_h may be due to one or a combination of the following sources:

- A physical process which is described exactly by an (unknown) operator F is modeled approximately by a computable linear operator T_h. Our analysis includes the important case that small nonlinearity effects are neglected in the mathematical model.
- $F = T \in L(X,Y)$ is approximated numerically by some operator T_h.
- For numerical computations finite dimensional subspaces $X_n \subset X$ and $Y_n \subset Y$ are needed, and $F = T$ is replaced by $Q_n T P_n$ where $P_n : X \to X_n$ and $Q_n : Y \to Y_n$ are projections.
- T_h is an integral operator with a kernel computed from measurement data.

In order to prove convergence rates under logarithmic source conditions with noisy operators, we need an analogue to the estimate

$$\frac{\pi}{4}\|S^\mu - \tilde{S}^\mu\| \le \|S - \tilde{S}\|^\mu, \tag{3.48}$$

which holds for positive, bounded, linear operators $S, \tilde{S}$, and $0 \le \mu \le 1$ (cf., e.g., [EHN96, §5.2]). This is provided by the following lemma:

Lemma 3.19. *Let $p > 0$ and $S, \tilde{S}$ positive linear operators in a Hilbert space X with $C := \sqrt{\|S\| + \|\tilde{S}\|} < 1$. Then the estimate*

$$\frac{\pi}{4}\|f_p(S) - f_p(\tilde{S})\| \le f_p(\|S - \tilde{S}\|) + f_p(\sqrt{C})\sqrt{\|S - \tilde{S}\|}$$

holds. Consequently, if $\|\tilde{S} - S\|$ is sufficiently small, then

$$\|f_p(S) - f_p(\tilde{S})\| \le 2 f_p\left(\|S - \tilde{S}\|\right). \tag{3.49}$$

Proof. Choose $n \in \mathbb{N}_0$ such that $0 < p < n+1$. Then the identity

$$\begin{aligned} A^{-p} &= C(p,n)\int_0^\infty t^{n-p}(tI+A)^{-n-1}\,\mathrm{d}t, \qquad (3.50)\\ C(p,n) &:= \frac{\sin p\pi}{\pi}\frac{n!}{(1-p)(2-p)\cdots(n-p)}, \end{aligned}$$

holds for any (unbounded) self-adjoint linear operator A with $\sigma(A) \subset [\sigma_0, \infty)$, $\sigma_0 > 0$ (cf. [KZPS76, §14]). By the spectral mapping theorem, (3.50) in particular holds for $A = -\ln S_{|X'}$. Here $X' := N(S)^\perp$, and $S(X') = X'$ since S is self-adjoint. For fixed $t \geq 0$, we have monotonically decreasing convergence of the functions

$$\left(t + \frac{1-\lambda^\mu}{\mu}\right)^{-n-1} \longrightarrow \begin{cases} (t - \ln\lambda)^{-n-1}, & 0 < \lambda \leq \|S\| \\ 0, & \lambda = 0 \end{cases}$$

as $\mu \searrow 0$. (To see this, note that $x \mapsto \frac{1-e^x}{x}$ is monotonically decreasing for $x \in \mathbb{R}$.) By Dini's theorem, convergence is uniform in λ. Hence it follows from the isometry of the functional calculus that

$$\begin{aligned} &\|(tI + \frac{1}{\mu}(I - S_{|X'}{}^\mu))^{-n-1} - (tI - \ln S_{|X'})^{-n-1}\| \\ = &\sup_{\lambda\in\sigma(S_{|X'})}\left|\left(t + \frac{1-\lambda^\mu}{\mu}\right)^{-n-1} - (t-\ln\lambda)^{-n-1}\right| \overset{\mu\searrow 0}{\to} 0. \end{aligned}$$

From this and the identity

$$(1-\lambda)^{-n-1} = \sum_{j=0}^\infty \binom{n+j}{n}\lambda^j$$

(with uniform convergence for $0 \leq \lambda \leq \|S\| < 1$), we obtain the representation

$$\begin{aligned} (tI - \ln S_{|X'})^{-n-1} &= \lim_{\mu\searrow 0}\left\{\left(\frac{t\mu+1}{\mu}I - \frac{1}{\mu}S_{|X'}{}^\mu\right)^{-n-1}\right\} \\ &= \lim_{\mu\searrow 0}\left\{\left(\frac{\mu}{t\mu+1}\right)^{n+1}\sum_{j=0}^\infty\binom{n+j}{n}\left(\frac{1}{t\mu+1}\right)^j S_{|X'}{}^{\mu j}\right\}. \end{aligned}$$

Convergence occurs in the operator norm. Plugging the last equation into (3.50) yields the identity

$$\begin{aligned} &f_p(S)x = C(p,n)\times \\ &\int_0^\infty t^{n-p}\lim_{\mu\searrow 0}\left\{\left(\frac{\mu}{t\mu+1}\right)^{n+1}\sum_{j=0}^\infty\binom{n+j}{n}\left(\frac{1}{t\mu+1}\right)^j S^{\mu j}x\right\}\,\mathrm{d}t \end{aligned}$$

for $x \in X' = N(S)^{\perp}$. Since this formula is trivially valid for $x \in N(S)$, it holds for all $x \in X$. Subtracting the corresponding formula for $\tilde{S}$, we obtain the estimate

$$\|f_p(S) - f_p(\tilde{S})\| \leq C(p,n) \times$$
$$\int_0^{\infty} t^{n-p} \lim_{\mu \searrow 0} \left\{ \left(\frac{\mu}{t\mu+1}\right)^{n+1} \sum_{j=0}^{\infty} \binom{n+j}{n} \left(\frac{1}{t\mu+1}\right)^j \left\| S^{\mu j} - \tilde{S}^{\mu j} \right\| \right\} \mathrm{d}t.$$

We first estimate the terms with $\mu j < 1$ on the right hand side, using (3.48):

$$\begin{aligned}
&\frac{\pi}{4} \left(\frac{\mu}{t\mu+1}\right)^{n+1} \sum_{j<\mu^{-1}} \binom{n+j}{n} \left(\frac{1}{t\mu+1}\right)^j \left\| S^{\mu j} - \tilde{S}^{\mu j} \right\| \\
&\leq \left(\frac{\mu}{t\mu+1}\right)^{n+1} \sum_{j=0}^{\infty} \binom{n+j}{n} \left(\frac{1}{t\mu+1}\right)^j \|S - \tilde{S}\|^{\mu j} \\
&= \left(t + \frac{1 - \|S - \tilde{S}\|^{\mu}}{\mu}\right)^{-n-1} \\
&\overset{\mu \searrow 0}{\to} \left(t - \ln \|S - \tilde{S}\|\right)^{-n-1}.
\end{aligned}$$

To estimate $\|S^{\mu j} - \tilde{S}^{\mu j}\|$ for $\mu j \geq 1$, we choose $M = 2^m$, $m \in \mathbb{N}$, such that $\frac{1}{2} \leq \frac{\mu j}{M} < 1$. It can be seen by induction on m that

$$\|S^M - \tilde{S}^M\| \leq (\|S\| + \|\tilde{S}\|)^{M-1} \|S - \tilde{S}\|.$$

Hence, by (3.48),

$$\frac{\pi}{4} \|S^{\mu j} - \tilde{S}^{\mu j}\| \leq \|S^M - \tilde{S}^M\|^{\frac{\mu j}{M}} \leq C^{\frac{M-1}{M}\mu j} \|S - \tilde{S}\|^{\frac{\mu j}{M}} \leq \sqrt{C}^{\mu j} \sqrt{\|S - \tilde{S}\|},$$

and we get

$$\begin{aligned}
&\frac{\pi}{4} \left(\frac{\mu}{t\mu+1}\right)^{n+1} \sum_{j \geq \mu^{-1}} \binom{n+j}{n} \left(\frac{1}{t\mu+1}\right)^j \left\| S^{\mu j} - \tilde{S}^{\mu j} \right\| \\
&\leq \left(\frac{\mu}{t\mu+1}\right)^{n+1} \sum_{j=0}^{\infty} \binom{n+j}{n} \left(\frac{\sqrt{C}^{\mu}}{t\mu+1}\right)^j \sqrt{\|S - \tilde{S}\|} \\
&= \left(\frac{\mu}{t\mu+1}\right)^{n+1} \left(1 - \frac{\sqrt{C}^{\mu}}{t\mu+1}\right)^{-n-1} \sqrt{\|S - \tilde{S}\|} \\
&\overset{\mu \searrow 0}{\to} \left(t - \ln \sqrt{C}\right)^{-n-1} \sqrt{\|S - \tilde{S}\|}.
\end{aligned}$$

Putting both estimates together finally gives

$$\frac{\pi}{4}\|f_p(S)-f_p(\tilde{S})\| \le C(p,n)\left(\int_0^\infty \frac{t^{n-p}\,\mathrm{d}t}{(t-\ln\|S-\tilde{S}\|)^{n+1}}+\right.$$
$$\left.+\int_0^\infty \frac{t^{n-p}\,\mathrm{d}t}{(t-\ln\sqrt{C})^{n+1}}\sqrt{\|S-\tilde{S}\|}\right)$$
$$= f_p(\|S-\tilde{S}\|)+f_p(C)\sqrt{\|S-\tilde{S}\|}.$$

■

We immediately obtain the following convergence result with an *a-priori* parameter choice rule.

Proposition 3.20. *Assume that the conditions (3.2), (3.10), (3.11), (3.19), (3.30), (3.46), and (3.47) are satisfied. Then the regularized solutions*

$$x_\alpha^{\delta,h} := g_\alpha(T_h^* T_h) T_h^* y^\delta \tag{3.51}$$

satisfy the error estimate

$$\|x_\alpha^{\delta,h} - x^\dagger\| \le C\left(\rho f_p(h) + \rho f_p(\alpha) + \frac{\delta + h\|x^\dagger\|}{\sqrt{\alpha}}\right).$$

In particular, for the choice $\alpha = h + \delta/\rho$ the estimate

$$\|x_\alpha^{\delta,h} - x^\dagger\| \le C\rho f_p\big((h+\delta/\rho)^2\big)$$

holds for $h + \delta/\rho$ sufficiently small.

Proof. With $x_\alpha^h := g_\alpha(T_h^* T_h) T_h^* y$ we have

$$\begin{aligned}
\|x^\dagger - x_\alpha^{\delta,h}\| &\le \|r_\alpha(T_h^*T_h)x^\dagger\| + \|g_\alpha(T_h^*T_h)T_h^*T_h x^\dagger - x_\alpha^{\delta,h}\| \\
&\le \|r_\alpha(T_h^*T_h)\|\cdot\|f_p(T^*T)w - f_p(T_h^*T_h)w\| \\
&\quad + \|r_\alpha(T_h^*T_h)f_p(T_h^*T_h)w\| + \|g_\alpha(T_h^*T_h)T_h^*\|\cdot\|T_h x^\dagger - y^\delta\|.
\end{aligned}$$

On the right hand side of this inequality, the first term is bounded by $C\rho f_p(h)$ due to (3.11), (3.49) and the estimate

$$\|T_h^*T_h - T^*T\| \le \|T_h^*(T_h - T)\| + \|(T_h^* - T^*)T\| \le \frac{2}{\mathrm{e}}h < h. \tag{3.52}$$

The second term is bounded by $C_1\rho f_p(\alpha)$ due to (3.30). Finally, we have

$$\|T_h x^\dagger - y^\delta\| \le \|T_h - F(x^\dagger)\| + \|y - y^\delta\| \le h\|x^\dagger\| + \delta, \tag{3.53}$$

due to (3.2) and (3.46), so by (3.15) the last term can be estimated by $C\alpha^{-1/2}(\delta + h\|x^\dagger\|)$. This gives the assertion. ■

We now consider a modification of an *a-posteriori* parameter choice rule suggested by Plato and Vainikko [PV90]. Let $Q_h : Y \to \overline{\operatorname{ran}(T_h)}$ be the orthogonal projection on $\overline{\operatorname{ran}(T_h)}$. We choose the regularization parameter α such that that following conditions are satisfied:

$$\|T_h x_\alpha^{\delta,h} - Q_h y^\delta\| \le 2\delta \max(-\ln\delta, 1) \quad \text{or} \quad \alpha = h \tag{3.54a}$$

$$h \le \alpha \le \exp(-1) \tag{3.54b}$$

$$\alpha < \exp(-1) \;\Rightarrow\; \begin{array}{l} \exists \alpha' \in [\alpha, 2\alpha] : \\ \|T_h x_{\alpha'}^{\delta,h} - Q_h y^\delta\| \ge 2\delta \max(-\ln\delta, 1) \end{array} \tag{3.54c}$$

We also consider the following alternative to (3.54c):

$$\alpha < \exp(-1) \;\Rightarrow\; \|T_h x_\alpha^{\delta,h} - Q_h y^\delta\| \ge \frac{3}{2}\delta \max(-\ln\delta, 1). \tag{3.54d}$$

Under the assumptions of Lemma 3.16 it can be shown that the algorithm

$$\begin{array}{l} n := 0, \qquad \alpha := \exp(-1) \\ \text{while } \left(\|T_h x_{\alpha_n}^{\delta,h} - Q_h y^\delta\| > 2\delta \max(-\ln\delta, 1) \text{ and } \alpha_n \ne h\right) \\ \qquad n := n + 1 \\ \qquad \text{if } (\alpha_n < \eta) \quad \alpha := h \\ \qquad \text{else} \quad \alpha := \alpha_n \end{array}$$

terminates after a finite number N of steps and yields a number $\alpha = \alpha_N$ satisfying (3.54a)-(3.54c) with $\alpha' = \alpha_{N-1}$ if $N > 0$.

To prove convergence rates with this parameter choice rule we need the following lemma.

Lemma 3.21. *For operators $T, T_h \in L(X,Y)$ with $\|T\|, \|T_h\| \le \exp(-1)$ and $\|T - T_h\| \le h$ the estimate*

$$\|T f_p(T^*T) - T_h f_p(T_h^* T_h)\| \le C\sqrt{h}$$

holds for some constant $C > 0$.

Proof. We use the polar decomposition $T = \tilde{T}|T|$. Here $|T| := (T^*T)^{1/2}$ is self-adjoint and $\tilde{T}$ is a partial isometry (cf., e.g., [Mur90]). Analogously, we have $T_h = \tilde{T}_h|T_h|$. By the triangle inequality, $\|\tilde{T}_h\| = 1$ (if $T_h \ne 0$), and $\|f_p(|T|^2)\| = \|f_p\|_{\infty,\sigma(|T|^2)} \le 1$ we obtain

$$\begin{aligned} \|T f_p(T^*T) - T_h f_p(T_h^*T_h)\| &= \|\tilde{T}|T| f_p(|T|^2) - \tilde{T}_h|T_h| f_p(|T_h|^2)\| \\ &\le \|(\tilde{T} - \tilde{T}_h)|T|\,\| \cdot \|f_p(|T|^2)\| + \|\tilde{T}_h\| \cdot \|\,|T| f_p(|T|) - |T_h| f_p(|T_h|^2)\| \\ &\le \|\tilde{T}|T| - \tilde{T}_h|T_h|\| + \|\tilde{T}_h\big(|T_h| - |T|\big)\| + \|\,|T| f_p(|T|^2) - |T_h| f_p(|T_h|^2)\|. \end{aligned}$$

By assumption, the first term on the right hand side of this inequality is bounded by h, and $h < \sqrt{h}$ since $h < 1$. To estimate the second term, we use (3.48) and obtain

$$\frac{\pi}{4}\| \, |T| - |T_h| \, \| \leq \sqrt{\|T^*T - T_h T_h^*\|} \leq \sqrt{h}.$$

To estimate the last term, we proceed as in the proof of Lemma 3.19 with $S := T^*T$ and $\tilde{S} := T_h^* T_h$ to establish the estimate

$$\|S^{1/2} f_p(S) - \tilde{S}^{1/2} f_p(\tilde{S})\| \leq C(p,n) \times$$
$$\int_0^\infty t^{n-p} \lim_{\mu \searrow 0} \left(\frac{\mu}{t\mu + 1}\right)^{n+1} \sum_{j=0}^{\infty} \binom{n+j}{n} \left(\frac{1}{t\mu+1}\right)^j \left\| S^{\mu j + \frac{1}{2}} - \tilde{S}^{\mu j + \frac{1}{2}} \right\| \, \mathrm{d}t.$$

If $\mu j + \frac{1}{2} \leq 1$, we have

$$\frac{\pi}{4}\left\| S^{\mu j + \frac{1}{2}} - \tilde{S}^{\mu j + \frac{1}{2}} \right\| \leq \|S - \tilde{S}\|^{\mu j} \sqrt{\|S - \tilde{S}\|} \leq C_1^{\mu j} \sqrt{\|S - \tilde{S}\|}$$

with $C_1 = \|S\| + \|\tilde{S}\| \leq 2\exp(-1)$ due to (3.48). If $\mu j + \frac{1}{2} > 1$, we choose $M \in \{2, 2^2, 2^3, \dots\}$ such that $\frac{1}{2} \leq \frac{\mu j + 1/2}{M} < 1$ to get

$$\begin{aligned}\frac{\pi}{4}\left\| S^{\mu j + \frac{1}{2}} - \tilde{S}^{\mu j + \frac{1}{2}} \right\| &\leq \|S^M - \tilde{S}^M\|^{\frac{\mu j + 1/2}{M}} \leq C_1^{\frac{M-1}{M}(\mu j + \frac{1}{2})} \|S - \tilde{S}\|^{\frac{\mu j + 1/2}{M}} \\ &\leq \sqrt{C_1} \sqrt{C_1}^{\mu j} \sqrt{\|S - \tilde{S}\|} \leq \sqrt{C_1}^{\mu j} \sqrt{\|S - \tilde{S}\|}.\end{aligned}$$

Proceeding as in the proof of Lemma 3.19, we obtain the desired estimate

$$\frac{\pi}{4}\|S^{1/2} f_p(S) - \tilde{S}^{1/2} f_p(\tilde{S})\| \leq f_p(\sqrt{C_1})\sqrt{h}.$$

This finishes the proof. ∎

Theorem 3.22. *Assume that the functions r_α and g_α satisfy (3.6), (3.10), (3.11) with $C_r = 1$, (3.34) with $\mu = 1/2$, and (3.32), that $x^\dagger$ satisfies a logarithmic source condition (3.19), that (3.46) and (3.47) hold, and that $\alpha = \alpha(\delta, h, y^\delta)$ is chosen such that (3.54a), (3.54b), and either (3.54c) or (3.54d) are satisfied. Then the estimate*

$$\|x_\alpha^{\delta,h} - x^\dagger\| \leq C\rho f_p(h) + \rho f_p\left((\sqrt{h} + \delta/\rho)^2\right)(1 + \mathrm{o}(1)). \tag{3.55}$$

holds for $\sqrt{h} + \delta/\rho$ sufficiently small with a constant C depending only on p and the regularization method.

Proof. Again, we assume w.l.o.g. that $\delta \leq \exp(-1)$. As in the proof of Proposition 3.20 we get the estimate

$$\|x^\dagger - x_\alpha^{\delta,h}\| \leq 2\rho f_p(h) + \|f_p(T_h^*T_h)r_\alpha(T_h^*T_h)w\| + C\frac{\delta + h\|x^\dagger\|}{\sqrt{\alpha}} \qquad (3.56)$$

1.) If $\alpha = \eta$, then the second term in (3.56) is bounded by $C_1\rho f_p(\eta)$ due to (3.30) which is a sufficient estimate. Let us assume that the other alternative in (3.54a) holds true. Proposition 3.6 with w replaced by $r_\alpha(T_h^*T_h)w$ yields

$$\|f_p(T_h^*T_h)r_\alpha(T_h^*T_h)w\| \leq \rho\sqrt{\phi_p^{-1}\left(\frac{\|T_h r_\alpha(T_h^*T_h)f_p(T_h^*T_h)w\|^2}{\rho^2}\right)}. \qquad (3.57)$$

From $C_r = 1$, (3.19), (3.47), (3.53) and Lemma 3.21 we obtain

$$\begin{aligned}
& \|T_h r_\alpha(T_h^*T_h)f_p(T_h^*T_h)w - Q_h(y^\delta - T_h x_\alpha^{\delta,h})\| \\
= \ & \|r_\alpha(T_hT_h^*)(T_h f_p(T_h^*T_h)w - Q_h y^\delta)\| \\
\leq \ & \|r_\alpha(T_hT_h^*)\| \cdot \|Q_h(T_h f_p(T_h^*T_h)w - y^\delta)\| \\
\leq \ & \|T_h f_p(T_h^*T_h)w - y^\delta\| \\
\leq \ & \|T_h f_p(T_h^*T_h)w - Tf_p(T^*T)w\| + \|Tx^\dagger - T_hx^\dagger\| + \|T_hx^\dagger - y^\delta\| \\
\leq \ & C\sqrt{h}\rho + 2h\|x^\dagger\| + \delta \leq C\sqrt{h}\rho + \delta.
\end{aligned}$$

Together with (3.54a) we obtain

$$\|T_h r_\alpha(T_h^*T_h)f_p(T_h^*T_h)w\| \leq (1 - 2\ln\delta)\delta + C\sqrt{h}\rho.$$

Plugging this into (3.57) yields

$$\|f_p(T_h^*T_h)r_\alpha(T_h^*T_h)w\| = \rho f_p\big((\sqrt{h} + \delta/\rho)^2\big)(1 + \mathrm{o}\,(1))$$

after a computation similar to (3.5.).

2.) We first assume that (3.54c) holds and show that the last term in (3.56) is $\mathrm{O}\,(f_{p+1}(\delta^2) + f_p(h))$. If $\sqrt{\alpha} \geq \delta/f_{p+1}(\delta)$ this follows immediately from (3.54b). Hence, we may assume that $\sqrt{\alpha} < \delta/f_{p+1}(\delta)$. Then, for δ sufficiently small, we obtain from (3.54c) that

$$\begin{aligned}
\|r_{\alpha'}(T_hT_h^*)T_hx^\dagger\| &\geq \|r_{\alpha'}(T_hT_h^*)Q_hy^\delta\| - \|Q_h(y^\delta - T_hx^\dagger)\| \\
&\geq \|Q_hy^\delta - T_hx_{\alpha',h}^\delta\| - \delta - h\|x^\dagger\| \\
&\geq \delta(-2\ln\delta - 1) - h\|x^\dagger\|.
\end{aligned}$$

Multiplying this inequality by $(\alpha')^{-1/2}$ and using Proposition 3.19, (3.32), (3.34) with $\mu = 1/2$, and (3.54b) yields

$$\begin{aligned}
\frac{\delta}{\sqrt{\alpha'}}(-\ln\delta^2 - 1) &\le \frac{1}{\sqrt{\alpha'}}\|r_{\alpha'}(T_h T_h^*)T_h x^\dagger\| + \frac{h}{\sqrt{\alpha'}}\|x^\dagger\| \\
&\le \frac{1}{\sqrt{\alpha'}}\|r_{\alpha'}(T_h T_h^*)T_h\big(f_p(T^*T) - f_p(T_h^*T_h)w\big)\| \\
&\quad + \frac{1}{\sqrt{\alpha'}}\|r_{\alpha'}(T_h T_h^*)T_h f_p(T_h^*T_h)w\| + \sqrt{2h}\|x^\dagger\| \\
&\le C f_p(h)\rho + f_p(\alpha')\rho + \sqrt{2h}\|x^\dagger\|.
\end{aligned}$$

Now we use our assumption on α to show that $f_p(\alpha') \le f_p(\delta^2)(1 + \mathrm{o}\,(1))$ (cf. (3.5.)) and divide by the last inequality by $(-\ln\delta^2 - 1)$. This yields $\delta/\sqrt{\alpha} \le \sqrt{2}\delta/\sqrt{\alpha'} = \mathrm{O}\,(f_{p+1}(\delta^2))$ and gives the desired estimate on the last term in (3.56). The proof with (3.54d) instead of (3.54c) is very similar. ■

3.7. Applications

We now give some examples of important inverse problems where the theory developed in this chapter is applicable.

3.7.1. Backwards Heat Equation

Problem 3.1. Let $\Omega \subset \mathbb{R}^m$ be a smooth (not necessarily bounded) domain, and let $u : \Omega \times (0, \bar{t}) \to \mathbb{R}$ satisfy the heat equation

$$\frac{\partial u}{\partial t} = \Delta u \qquad \text{in } \Omega \times (0, \bar{t}) \tag{3.58}$$

and the initial condition

$$u(\cdot, 0) = f \tag{3.59}$$

for some $f \in L^2(\Omega)$. If $\Omega \ne \mathbb{R}^m$, we additionally impose one of the boundary conditions

$$u = 0 \qquad \text{on } \partial\Omega \times (0, \bar{t}] \tag{3.60}$$

or

$$\frac{\partial u}{\partial \nu} = 0 \qquad \text{on } \partial\Omega \times (0, \bar{t}]. \tag{3.61}$$

The problem is to identify the initial values f from measurements of the final values

$$g := u(\cdot, \bar{t}).$$

To analyze this problem, let us first collect some facts about unbounded operators in Hilbert spaces. Recall that a linear operator $A : X \supset \mathcal{D}(A) \to X$ is *self-adjoint* if it is symmetric, i.e. $\langle Ax, y \rangle = \langle x, Ay \rangle$ for all $x, y \in \mathcal{D}(A)$ and if $\mathcal{D}(A) = \mathcal{D}(A^*)$, $\mathcal{D}(A^*) := \{x \in X : \exists z \in X \forall y \in \mathcal{D}(A)\, \langle x, Ay \rangle = \langle z, y \rangle\}$. For unbounded operators the latter condition is usually much harder to check than the former. However, the spectral theorem only holds for self-adjoint, not for symmetric operators. It can be shown (but the proofs are not easy!) that the Laplace operator Δ is self-adjoint on either of the domains

$$\mathcal{D}(\Delta) = \{v \in H^2(\Omega) : v = 0 \text{ on } \partial\Omega\}, \tag{3.62}$$

and

$$\mathcal{D}(\Delta) = \{v \in H^2(\Omega) : \frac{\partial v}{\partial \nu} = 0 \text{ on } \partial\Omega\} \tag{3.63}$$

(cf. [Tay96, §8.2]). Of course, the boundary conditions have to be understood in the sense of the trace operator. For $\Omega = \mathbb{R}^m$, Δ is self-adjoint on the domain $\mathcal{D}(\Delta) = H^2(\mathbb{R}^m)$.

We interpret (3.58) as an ordinary differential equation for the vector-valued function $t \mapsto u(\cdot, t)$, $[0, \bar{t}] \to L^2(\Omega)$ with initial condition (3.59) and require that

$$u(\cdot, t) \in \mathcal{D}(\Delta), \qquad 0 < t < \bar{t}. \tag{3.64}$$

With (3.62) or (3.63), this takes care of the boundary condition (3.60) or (3.61), rsp., and (3.58) makes sense as an ODE. The solution is easily found to be

$$u(\cdot, t) = \exp(t\Delta) f, \qquad t \in [0, \bar{t}]$$

(cf. [RR92] or [Paz83]). We interpret this formula in the sense of the functional calculus for unbounded self-adjoint operators. Note that (3.64) is satisfied since $\Delta \le 0$ and $\sup_{\lambda \le 0} |\lambda \exp(t\lambda)| < \infty$ for $t > 0$.

We can now formulate Problem 3.1 as an operator equation of the form (3.1) with $X = Y = L^2(\Omega)$ and $T = T_{\mathrm{BH}}$ given by

$$T_{\mathrm{BH}} := \frac{1}{\sqrt{\mathrm{e}}} \exp(\bar{t}\Delta).$$

The scaling factor $1/\sqrt{\mathrm{e}}$ has been introduced to meet (3.19b).

Proposition 3.23. *For Problem 3.1, condition 3.19 has the interpretation*

$$\operatorname{ran}\Big(f_p(T_{\mathrm{BH}}^* T_{\mathrm{BH}})\Big) = \mathcal{D}\Big((I-\Delta)^p\Big).$$

Proof. We have

$$f_p(T_{\mathrm{BH}}^* T_{\mathrm{BH}}) = \left(f_p \circ \frac{1}{\mathrm{e}} \exp 2\bar{t}\cdot\right)(\Delta) = (I - 2\bar{t}\Delta)^{-p}.$$

Since there are constants $c, C > 0$ such that $c(1+\lambda)^p \le (1+2\bar{t}\lambda)^p \le C(1+\lambda)^p$ for all $\lambda \ge 0$, it follows that

$$\begin{aligned}
\mathcal{D}\Big((I-\Delta)^p\Big) &= \left\{v \in L^2(\Omega) : \int_0^\infty (1+\lambda)^{2p}\, \mathrm{d}\|E_\lambda v\|^2 < \infty\right\} \\
&= \left\{v \in L^2(\Omega) : \int_0^\infty (1+2\bar{t}\lambda)^{2p}\, \mathrm{d}\|E_\lambda v\|^2 < \infty\right\} \\
&= \mathcal{D}\Big((I-2\bar{t}\Delta)^p\Big) = \operatorname{ran}\Big(f_p(T_{\mathrm{BH}}^* T_{\mathrm{BH}})\Big).
\end{aligned}$$

Here $\{E_\lambda\}$ is the spectral family of the positive, self-adjoint operator $-\Delta$. ■

Remark 3.24. If $\Omega = \mathbb{R}^m$, then

$$\mathcal{D}((I-\Delta)^p) = H^{2p}(\Omega). \tag{3.65}$$

With boundary conditions the situation becomes more complicated. Neubauer [Neu88] has shown that (3.65) cannot hold if Ω is bounded (and under weak additional assumptions, (3.65) cannot hold even if $I-\Delta$ is replaced by some other self-adjoint, densely defined, strictly positive operator).

For $p \in \mathbb{N}$, we have

$$\mathcal{D}\Big((I-\Delta)^p\Big) = \{v \in H^{2p}(\Omega) : \Delta^q v = 0 \text{ on } \partial\Omega \text{ for } q = 0, 1, \ldots, p-1\}$$

in case of Dirichlet boundary conditions and

$$\mathcal{D}\Big((I-\Delta)^p\Big) = \{v \in H^{2p}(\Omega) : \frac{\partial \Delta^q v}{\partial \nu} = 0 \text{ on } \partial\Omega \text{ for } q = 0, 1, \ldots, p-1\}$$

in case of Neumann boundary conditions.

3.7.2. An inverse problem in satellite gradiometry

Problem 3.2. Let u satisfy the Laplace equation

$$\Delta u = 0 \qquad \text{in } \{x \in \mathbb{R}^{m+1} : |x| > 1\}.$$

For $m = 2$, u describes the gravitational potential of the earth in a spherical framework when the radius of the earth has been normalized to 1. The behavior of u at infinity is described by

$$|u(x)| = \mathrm{O}\left(|x|^{1-m}\right), \qquad |x| \to \infty.$$

The problem is to determine the potential

$$f = u\big|_{S^m}$$

at the surface $S^m := \{x \in \mathbb{R}^{m+1} : |x| = 1\}$ of the earth from satellite measurements of

$$g = \frac{\partial^2 u}{\partial r^2}\bigg|_{RS^m} \qquad (r = |x|)$$

at $RS^m = \{x \in \mathbb{R}^{m+1} : |x| = R\}$, $R > 1$. Here $-\nabla u$ describes the gravitational force and $-\frac{\partial^2 u}{\partial r^2}$ the rate of change of the gravitational force in radial direction.

Let v be the solution to the interior Laplace equation with Dirichlet boundary values f. With $r = |x|$ and $\hat{x} = x/|x|$, v is given by the Poisson formula

$$v(r\hat{x}) = v(\hat{x}, r) = \frac{1 - r^2}{\gamma_m} \int_{S^m} \frac{f(\hat{y})\,\mathrm{d}s(y)}{|r\hat{x} - \hat{y}|^{m+1}}, \tag{3.66}$$

where $\gamma_m = 2\pi^{(m+1)/2}/\Gamma((m+1)/2)$ is the surface area of S^m. An elementary calculation using the formula

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{m+1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta_{S^m} \tag{3.67}$$

(cf. (1.33)) yields

$$u(\hat{x}, r) = r^{1-m} v(\hat{x}, \frac{1}{r}).$$

Thus, we may formulate Problem 3.2 as a first kind integral equation of the form (3.1) with $T = T_{\mathrm{SG}} : L^2(S^m) \to L^2(S^m)$ given by

$$(T_{\mathrm{SG}} f)(\hat{x}) = \frac{c}{\gamma_m} \int_{S^m} \frac{\partial^2}{\partial R^2} \left\{ R^{1-m} \frac{1 - R^{-2}}{|R^{-1}\hat{x} - \hat{y}|^{m+1}} \right\} f(\hat{y})\,\mathrm{d}s(\hat{y}).$$

Here the scaling constant c is chosen such that (3.19b) is fulfilled. Note that T_{SG} has an infinitely smooth kernel and thus maps $L^2(S^m)$ to $C^\infty(S^m)$. This indicates that Problem 3.2 is severely ill-posed. The next proposition shows that again logarithmic sources conditions are smoothness conditions in terms of Sobolev spaces.

Proposition 3.25. *For Problem 3.2, condition (3.19) has the interpretation*

$$\operatorname{ran}\left(f_p(T_{\mathrm{SG}}^* T_{\mathrm{SG}})\right) = H^p(S^m).$$

Proof. In analogy to the analysis in §3.7.1. we interpret the Laplace equation with formula (3.67) for the Laplacian as a second order ODE in r with an initial condition at $r = 1$. We obtain two solutions, one defined for $r \geq 1$, the other one for $0 < r \leq 1$:

$$\begin{aligned} & u(\cdot, r) = r^{-(m-1)/2} r^{-\Lambda} f, \qquad v(\cdot, r) = r^{-(m-1)/2} r^{\Lambda} f, \\ & \Lambda := \left(-\Delta_{S^m} + \left(\frac{m-1}{2}\right)\right)^{1/2} \end{aligned}$$

This implies

$$\frac{\partial^2}{\partial r^2} u(\cdot, r) = \left(-\frac{m-1}{2} - \Lambda\right)\left(-\frac{m+1}{2} - \Lambda\right) r^{-\frac{m+3}{2} - \Lambda} f,$$

i.e.

$$T_{\mathrm{SG}}^* T_{\mathrm{SG}} = \chi(\Lambda), \quad \chi(\lambda) := c^2 \left(-\frac{m-1}{2} - \lambda\right)^2 \left(-\frac{m+1}{2} - \lambda\right)^2 R^{-(m+3)-2\lambda}.$$

An easy calculation shows that

$$\frac{1}{f_p(\chi(\lambda))} = \Big(-\ln(\chi(\lambda))\Big)^p = (\ln R^2)\lambda^p + \Xi(\lambda)$$

where $\Xi(\lambda)$ is bounded for $\lambda \in [\frac{m-1}{2}, \infty) \supset \sigma(\Lambda)$. It follows that

$$\begin{aligned} \operatorname{ran}\left(f_p(T_{\mathrm{SG}}^* T_{\mathrm{SG}})\right) &= \operatorname{ran}\Big((f_p \circ \chi)(\Lambda)\Big) = \mathcal{D}\Big((\ln R^2)\Lambda^p + \Xi(\Lambda)\Big) \\ &= \mathcal{D}(\Lambda^p) = H^p(S^m). \end{aligned}$$

■

3.7.3. Sideways Heat Equation

Problem 3.3. Let $u : [0,1] \times \mathbb{R} \to \mathbb{C}$ satisfy the heat equation

$$u_t(t,x) = u_{xx}(t,x).$$

The interval $[0,1]$ represents some heat conducting medium (e.g. the wall of a furnace) where one side ($x = 0$) is accessible and the other one is not. We assume the accessible side to be insulated, i.e.

$$u_x(0,t) = 0, \qquad t \in \mathbb{R}.$$

The problem is to determine the temperature at the inaccessible side

$$g = u(1,\cdot)$$

from measurements of the temperature at the accessible side

$$f = u(0,\cdot).$$

We make a Fourier transform in the time variable, i.e. we consider

$$(\mathcal{F}u)(x,\omega) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\langle\omega,t\rangle} u(x,t)\,\mathrm{d}t.$$

Under appropriate smoothness assumptions we have

$$\mathcal{F}u_{xx} = (\mathcal{F}u)_{xx} \qquad \text{and} \qquad \mathcal{F}u_t = \mathrm{i}\omega\mathcal{F}u.$$

Hence, $\mathcal{F}u$ is characterized by the equations

$$\begin{aligned}(\mathcal{F}u)_{xx} &= \mathrm{i}\omega\mathcal{F}u,\\ (\mathcal{F}u)_x(0,\cdot) &= 0,\\ (\mathcal{F}u)(1,\cdot) &= \mathcal{F}f.\end{aligned}$$

These equations are easily solved explicitly. We get

$$(\mathcal{F}u)(x,\omega) = \frac{\cosh\sqrt{\mathrm{i}\omega}x}{\cosh\sqrt{\mathrm{i}\omega}}(\mathcal{F}f)(\omega)$$

with $\sqrt{\mathrm{i}\omega} = \sqrt{\frac{\omega}{2}} + \mathrm{i}\sqrt{\frac{\omega}{2}}$. Therefore, we describe Problem 3.3 by an operator equation (3.1) with $X = Y = L^2(\mathbb{R})$ and

$$T_{\mathrm{SH}} := \mathcal{F}^{-1}c(\cosh\sqrt{\mathrm{i}\omega})^{-1}\mathcal{F}. \tag{3.68}$$

Here $c(\cosh\sqrt{\mathrm{i}\omega})^{-1}$ denotes a multiplication operator, and we have introduced a scaling constant $c := \exp(-1/2)\inf_\omega|\cosh\sqrt{\mathrm{i}\omega}| > 0$ to meet (3.19b).

Proposition 3.26. *For Problem 3.2, condition (3.19) has the interpretation*

$$\operatorname{ran}\left(f_p(T_{\mathrm{SH}}^* T_{\mathrm{SH}})\right) = H^{p/2}(\mathbb{R}).$$

Proof. If $A : X \to X$ is some self-adjoint operator and $W : Y \to X$ a unitary operator, then the functional calculus of A and $W^{-1}AW$ are related by

$$f(W^{-1}AW) = W^{-1} f(A) W. \tag{3.69}$$

(To see this, note that $\{W^{-1}E_\lambda W\}$ is the spectral family of $W^{-1}AW$ if $\{E_\lambda\}$ is the spectral family of A.) With $W = \mathcal{F}$ and $A = T_{\mathrm{SH}}^* T_{\mathrm{SH}} = \mathcal{F}^{-1} c^2 |\cosh \sqrt{\mathrm{i}\omega}|^{-2} \mathcal{F}$, this implies

$$\operatorname{ran}\left(f_p(T_{\mathrm{SH}}^* T_{\mathrm{SH}})\right) = \left\{ \varphi \in L^2(\mathbb{R}) : \frac{1}{f_p(c^2 |\cosh \sqrt{\mathrm{i}\omega}|^{-2})} \mathcal{F}\varphi \in L^2(\mathbb{R}) \right\}.$$

From

$$|\cosh \sqrt{\mathrm{i}\omega}|^2 = \sinh^2 \sqrt{\frac{\omega}{2}} + \cos^2 \sqrt{\frac{\omega}{2}}$$

it is easily seen that

$$-\ln c^2 |\cosh \sqrt{\mathrm{i}\omega}|^{-2} \sim (1+\omega^2)^{1/4}$$

and

$$\frac{1}{f_p((c^2 |\cosh \sqrt{\mathrm{i}\omega}|)^{-2})} \sim (1+\omega^2)^{p/4}$$

in the sense that the left hand side is bounded from above and below by constant multiples of the right hand side with positive constants independent of ω. Hence,

$$\operatorname{ran}\left(f_p(T_{\mathrm{SH}}^* T_{\mathrm{SH}})\right) = \left\{ \varphi \in L^2(\mathbb{R}) : (1+|\omega|^2)^{p/4} \mathcal{F}\varphi \in L^2(\mathbb{R}) \right\} = H^{p/2}(\mathbb{R}).$$

∎

Remark 3.27. From (3.68), (3.69), and $D = \mathcal{F}^{-1} \omega \mathcal{F}$, $D := \frac{1}{i}\frac{d}{dt}$, it follows that

$$T_{SH}^* T_{SH} = c^2 |\cosh \sqrt{\mathrm{i}D}|^{-2}.$$

4. Iterative regularization of nonlinear exponentially ill-posed problems

In the last few years quite a number of iterative regularization methods for nonlinear ill-posed problems have been suggested. After giving a definition of the term iterative regularization method, we describe some typical examples of this class of methods and review some convergence results. Due to fast convergence, regularized Newton methods are particularly attractive. *Convergence rates* for nonlinear exponentially ill-posed problems have first been shown in [Hoh97] for the iteratively regularized Gauß-Newton method (IRGNM), and in [DES98] for Landweber iteration. Here we suggest a generalization of the IRGNM where iterated Tikhonov regularization is used to solve the linearized problem and give a convergence rates analysis under logarithmic source conditions. In the next chapter we will see that this generalization of the IRGNM yields better numerical results. Finally, we apply the abstract theory to an inverse potential and to inverse obstacle problems, and we show that the logarithmic source conditions are essentially equivalent to smoothness conditions in Sobolev spaces.

4.1. Introduction to iterative regularization methods

We consider the following abstract setting: Let X and Y be Hilbert spaces, and $F : X \supset D(F) \to Y$ a nonlinear operator that is continuously Fréchet differentiable on its domain $D(F)$. We want to solve the operator equation

$$F(x) = y. \tag{4.1}$$

Let $x^\dagger$ be an exact solution, i.e. $F(x^\dagger) = y$. We assume that only noisy data y^δ are available satisfying

$$\|y^\delta - y\| \leq \delta \tag{4.2}$$

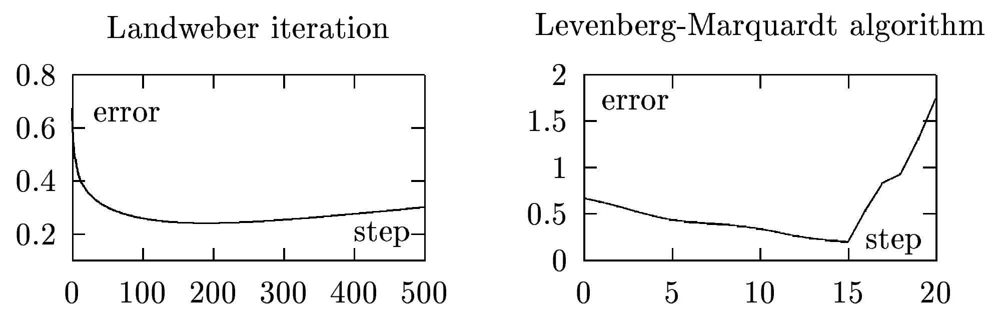


Figure 4.1: Semiconvergence; 10% data noise error

with some known noise level δ.

Definition 4.1. An iterative method $x_{n+1}^\delta := \Phi(x_n^\delta, \dots, x_0, y^\delta)$ together with a stopping rule $N(\delta, y^\delta)$ is called an *iterative regularization method* for F if for all $x^\dagger \in D(F)$, $y := F(x^\dagger)$, all y^δ satisfying (4.2) and all initial guesses x_0 sufficiently close to $x^\dagger$ the following conditions hold:

- x_n^δ is well defined for $n = 1, \dots, N(\delta, y^\delta)$, and $N(\delta, y^\delta) < \infty$ for $\delta > 0$.
- For exact data ($\delta = 0$) either $N = N(\delta, y^\delta) < \infty$ and $x_N^\delta = x^\dagger$ or $N = \infty$ and $\|x_n - x^\dagger\| \to 0$ for $n \to \infty$.
- The following regularization property holds:

$$\sup_{\|y^\delta - y\| \le \delta} \|x^\delta_{N(\delta, y^\delta)} - x^\dagger\| \to 0, \qquad \delta \to 0. \tag{4.3}$$

The choice of the stopping index is a very important issue for iterative regularization methods since typically the approximations deteriorate quite rapidly for noisy data after a certain number of iterations (cf. Fig. 4.1). The most well-known stopping rule is the *discrepancy principle* which consists in stopping the iteration at the first index $N = N(\delta, y^\delta)$ for which

$$\|F(x_N) - y^\delta\| \le \tau\delta \tag{4.4}$$

with some fixed constant $\tau > 1$.

Landweber iteration Landweber iteration is defined by the formula

$$x_{n+1}^\delta := x_n^\delta + \mu F'[x_n^\delta]^*(y^\delta - F(x_n^\delta)). \tag{4.5}$$

μ is a scaling parameter that has to be chosen such that $\|F'[x]\| \le 1/\mu$ for all x in a neighborhood of $x^\dagger$. Hanke, Neubauer, and Scherzer [HNS95] have proved the following result:

Theorem 4.2. *If the nonlinearity condition*

$$\|F(x) - F(\bar{x}) - F'[x](x - \bar{x})\| \leq \eta \|F(x) - F(\bar{x})\| \tag{4.6}$$

holds for all $x, \bar{x}$ *in a neighborhood of* $x^\dagger$ *and some* $\eta < \frac{1}{2}$, *then Landweber iteration together with the discrepancy principle with* $\tau > 2\frac{1+\eta}{1-2\eta}$ *is a regularization method in the sense of Definition 4.1.*

In [DES98] an estimate

$$\|x_n^\delta - x^\dagger\| \leq C(\ln n)^{-p}, \qquad n \leq N(\delta, y^\delta) \tag{4.7}$$

and order optimal convergence rates have been shown under logarithmic source conditions and the *Newton- Mysovskii condition*

$$\|(F'[x] - F'[x^\dagger])F'[x^\dagger]^{-1}\| \leq C\|x - x^\dagger\|, \qquad x \in D(F). \tag{4.8}$$

(For linear problems this follows from the theory presented in Chapter 3.) Moreover, the estimate $N = O\left((-\ln \delta)^{-2p}/\delta^2\right)$ for the number of iterations has been derived. Unfortunately, it can be shown that the Newton-Mysovskii condition is not satisfied for the applications considered in Section 4.4.. The conditions (4.6) and (4.13), (4.18) below could neither be proven to be true or false (cf. Section 4.5.).

Inexact Newton methods In inexact Newton methods, the linearized equation

$$F'[x_n^\delta]h_n + F(x_n^\delta) = y^\delta \tag{4.9}$$

is considered to compute an update $h_n = x_{n+1}^\delta - x_n^\delta$. As (4.9) typically inherits the ill-posedness from the nonlinear problem, it has to be regularized. In principle any regularization method discussed in Chapter 3 can be used to find an approximate solution to (4.9). This leads to formulae of the form

$$x_{n+1}^\delta := x_n^\delta + g_n(A_n^* A_n) A_n^* (y^\delta - F(x_n^\delta)) \tag{4.10}$$

where $A_n := F'[x_n^\delta]$ and $g_n(\lambda) \approx 1/\lambda$.

For Tikhonov regularization we have $g_n(\lambda) = 1/(\lambda + \alpha_n)$. Then the updates $h_n \in X$ solve the minimization problems

$$\|A_n h + F(x_n^\delta) - y^\delta\|^2 + \alpha_n \|h\|^2 = \min! \tag{4.11}$$

This is the *Levenberg-Marquardt algorithm*. A convergence analysis was given by Hanke [Han97a] under the assumption that the regularization parameters α_n are chosen such that

$$\|A_n h_n + F(x_n^\delta) - y^\delta\| = \rho \|F(x_n^\delta) - y^\delta\| \tag{4.12}$$

with some $\rho < 1$ and that the discrepancy principle (4.4) with $\tau > 1/\rho$ is used to stop the iteration.

Another possibility is to use iterative methods to find a regularized solution to (4.9). If the adjoint $F'[x_n^\delta]^*$ can be computed directly as for inverse scattering problems (cf. Section 4.4.), these methods have the advantage that a costly computation and inversion of the matrix for A_n is avoided. A particularly attractive choice of the inner iteration is the conjugate gradient method for the normal equation (CGNE) (cf. Fig. 4.2). This method requires the fewest iterations among all semi-iterative methods if the discrepancy principle

$$\|A_n h_n + F(x_n^\delta) - y^\delta\| \le \rho \|F(x_n^\delta) - y^\delta\|$$

is used as stopping rule for the inner iteration (cf. [EHN96]). Since g_n is a polynomial which depends on the right hand side, the CGNE is a nonlinear regularization method for linear problems. The Newton-CG method has also been investigated by Hanke [Han97b]. He suggested to stop the outer iteration by (4.4) with $\tau > 2/\rho^2$.

Theorem 4.3. *Let F satisfy the nonlinearity condition*

$$\|F(x) - F(\bar{x}) - F'[x](x - \bar{x})\| \le c\|x - \bar{x}\|\|F(x) - F(\bar{x})\| \tag{4.13}$$

for all $x, \bar{x}$ in a neighborhood of $x^\dagger$. Then the versions of the Levenberg-Marquardt algorithm and the Newton-CG method described above are regularization methods in the sense of Definition 4.1.

Rieder [Rie99] has proved convergence rates for inexact Newton methods with linear regularization methods (e.g. Tikhonov regularization, Landweber iteration or ν-methods, but not CGNE) under Hölder-type source conditions with $\mu > \frac{1}{2}$ and the nonlinearity condition

$$F'[\bar{x}] = R(\bar{x}, x)F'[x] \qquad \text{and} \qquad \|I - R(\bar{x}, x)\| \le C_R\|x - \bar{x}\|.$$

Unfortunately, his techniques cannot be applied for weaker sources conditions such as Hölder-type source conditions with $\mu \le \frac{1}{2}$ or logarithmic source conditions.

InexactNewton(out : x; in : x_0, y^δ)
$n = 0$
while $\|y^\delta - F(x_n)\| > \tau\delta$
  begin
  CGNE($h_n, y^\delta - F(x_n), 0$)
  $x_{n+1} = x_n + h_n$
  $n = n + 1$
  end
$x = x_n$

Bakushinskii(out : x; in : x_0, y^δ)
$n = 0$
while $\|y^\delta - F(x_n)\| > \tau\delta$
  begin
  CGNE($h_n, y^\delta - F(x_n), x_0 - x_n$)
  $x_{n+1} = x_n + h_n$
  $n = n + 1$
  end
$x = x_n$

CGNE(out : h; in : z, h_0)
$k = 0$
$r_0 = z - F'[x_n]h_0$
$d_1 = s_0 = F'[x_n]^* r_0$
repeat
  $q_{k+1} = F'[x_n]d_{k+1}$
  $\alpha_{k+1} = \|s_k\|^2 / \|q_{k+1}\|^2$
  $h_{k+1} = h_k + \alpha_{k+1} d_{k+1}$
  $r_{k+1} = r_k - \alpha_{k+1} q_{k+1}$
  $s_{k+1} = F'[x_n]^* r_{k+1}$
  $\beta_{k+1} = \|s_{k+1}\|^2 / \|s_k\|^2$
  $d_{k+1} = s_{k+1} + \beta_{k+1} d_k$
  $k = k + 1$
until ($\|r_k\| < \rho\|z\|$ or $k \geq k_{\max}$)
$h = h_k$

Figure 4.2: Inexact Newton and Bakushinskii methods with CGNE as inner iteration

Second Degree methods Recently, Hettlich and Rundell [HR] have suggested a class of methods that use the second derivative of the operator F. A predictor-corrector procedure is used to avoid solving quadratic equations. The predictor $\tilde{h}_n$ is computed by a formula similar to (4.10). Then, the corrector h_n is obtained as a regularized solution of the linear equation

$$A_n h_n + \frac{1}{2} F''[x_n^\delta](h_n, \tilde{h}_n) = y^\delta - F(x_n^\delta).$$

The authors used Tikhonov regularization with constant regularization parameter in both the predictor and the corrector step. The following convergence result was shown:

Theorem 4.4. *The second degree method described above with the stopping rule (4.4) is a regularization method in the sense of Definition 4.1 if (4.13) holds, $\|F'\|$, and $\|F''\|$ are locally bounded, and if τ and the regularization parameter in the corrector step are chosen sufficiently large.*

Numerical experiments reported in [HR] show that better reconstructions are obtained in the first iteration steps, but the asymptotic behavior is the same as that of the Levenberg-Marquardt algorithm.

Bakushinskii methods Another class of iterative regularization methods is given by the recursion formula

$$x_{n+1}^\delta \;:=\; x_0 + g_n(A_n^* A_n) A_n^* \Big(y^\delta - F(x_n^\delta) + A_n(x_n^\delta - x_0) \Big). \tag{4.14}$$

If F is linear, then the terms $F(x_n^\delta)$ and $A_n x_n^\delta$ cancel out, and (4.14) reduces to the linear regularization method described by g_n provided with initial guess x_0. In this case the results from previous iterations are not used at all. Unlike for inexact Newton methods, standard linear theory immediately yields convergence results for method (4.14) in the linear case. (An exception is the Levenberg-Marquardt algorithm with $\alpha_n = const$ which reduces to *Lardy's method* in the linear case. Convergence results for Lardy's method are well known.)

We will see in the next sections that the total error $x_n^\delta - x^\dagger$ for the iteration (4.14) can be separated into components corresponding to the linearized equation and components due to the nonlinearity of F. Both error components can be estimated separately which makes the iteration (4.14) easier to analyze than (4.10).

The choice $g_n(\lambda) := \frac{1}{\alpha_n + \lambda}$ in (4.14) yields the *iteratively regularized Gauß-Newton method* (IRGNM) suggested by Bakushinskii [Bak92]. Bakushinskii provided a convergence rates analysis of this method for the Hölder source condition with $\mu = 1$ and the condition that the regularization parameters α_n satisfy

$$\lim_{n\to\infty} \alpha_n = 0 \quad \text{and} \quad 1 \leq \frac{\alpha_n}{\alpha_{n+1}} \leq \gamma \tag{4.15}$$

for all $n \in \mathbb{N}_0$ with some $\gamma > 1$. We will often work with the simple choice

$$\alpha_n = \alpha_0 \gamma^{-n}. \tag{4.16}$$

Using the substitution $\bar{h} = h + x_n^\delta - x_0$ it is easily seen that the updates $h_n = x_{n+1}^\delta - x_n^\delta$ solve the minimization problems

$$\|A_n h + F(x_n^\delta) - y^\delta\|^2 + \alpha_n \|h + x_n^\delta - x_0\|^2 = \min! \tag{4.17}$$

The additional term $x_n^\delta - x_0$ compared to (4.11) has an additional regularizing effect since it prevents the iterates x_{n+1}^δ from getting too far away from the initial guess x_0.

The following result was shown by Blaschke/Kaltenbacher, Neubauer and Scherzer [BNS97]:

Theorem 4.5. *The IRGNM with the discrepancy principle is a regularization method under the nonlinearity condition*

$$\begin{aligned} &F'[\bar{x}] = R(\bar{x}, x)F'[x] + Q(\bar{x}, x) \\ &\|I - R(\bar{x}, x)\| \leq C_R, \quad \|Q(\bar{x}, x)\| \leq C_Q \|F'[x^\dagger](\bar{x} - x)\| \end{aligned} \tag{4.18}$$

for $\|x - x^\dagger\|, \|\bar{x} - x^\dagger\| \leq E$, $E > 0$.

Moreover, the authors of [BNS97] proved order optimal convergence rates for Hölder-type source conditions with $0 < \mu \leq 1/2$. We will see below that the IRGNM also converges of optimal order under *logarithmic* source conditions and that

$$\|x_n^\delta - x^\dagger\| \leq C f_p(\alpha_n) \tag{4.19}$$

for $n \leq N(\delta, y^\delta)$ with $N(\delta, y^\delta) = \mathrm{O}(-\ln \delta)$ in this case.

Another attractive choice for the function g_n in (4.14) is

$$g_n^l(\lambda) := \frac{(\lambda + \alpha_n)^l - \alpha_n^l}{\lambda(\lambda + \alpha_n)^l}, \qquad l \in \mathbb{N}, \tag{4.20}$$

which corresponds to iterated Tikhonov regularization. The implementation of one iteration step is similar to linear iterated Tikhonov regularization:

$$\begin{aligned} & h_1 := \text{solution to (4.17)} \\ & \text{for } (j = 2, \dots, l) \\ & \quad h_j := \operatorname{argmin}_{h \in X} (\|A_n h + F(x_n^\delta) - y^\delta\|^2 + \alpha_n \|h - h_{j-1}\|^2) \\ & x_{n+1}^\delta := x_n^\delta + h_l \end{aligned} \tag{4.21}$$

Note that the computation of $h_2, \dots, h_l$ is very cheap since the same matrix has to be inverted as in the first inner step and since there is no further operator evaluation. Roughly speaking, one gets the effect of almost l Newton steps for the cost of a little more than one. To our knowledge this method has not been investigated previously. A convergence rates analysis under logarithmic source conditions is given in Theorem 4.7 below.

Just as in (4.10) it is also possible to use an iterative method in (4.14). In comparison to (4.10) this amounts to using $x_0 - x_n^\delta$ instead of 0 as initial guess for the inner iteration (cf. Fig. 4.2). The CGNE iteration in Fig. 4.2 can be replaced, e.g., by Landweber iteration or a ν-method. A convergence rates analysis of (4.14) with Landweber iteration was given by Blaschke/-Kaltenbacher [Kal97], [Kal98] under Hölder-type source conditions.

4.2. A convergence theorem for operator perturbations and an a-priori rule

In this section we present a convergence result for the IRGNM with an a-priori parameter choice rule. We assume that in the nth iteration step the operator F is approximated numerically by an operator $F^{(n)}$ with $D(F^{(n)}) \supset D(F)$ such that the estimate

$$\|F^{(n)}(x_n^\delta) - F(x_n^\delta)\| \le f_p(h_n) h_n \tag{4.22a}$$

is satisfied for some error level $h_n \ge 0$ (cf. 3.18). Moreover, we assume that $F^{(n)}$ is Fréchet differentiable and that the derivative of $F^{(n)}$ at x is approximated by an operator $A_x^{(n)}$ such that

$$\|A_x^{(n)} - F'[x]\| \le h_n \tag{4.22b}$$

$$\|A_x^{(n)} - F^{(n)\prime}[x]\| \le h_n \tag{4.22c}$$

for all x in a neighborhood of $x^\dagger$. Thus, writing $A_n^{(n)}$ for $A_{x_n^\delta}^{(n)}$, we consider the recursion formula

$$x_{n+1}^\delta := x_0 + g_n^l \left(A_n^{(n)*} A_n^{(n)} \right) A_n^{(n)*} \left(y^\delta - F^{(n)}(x_n^\delta) + A_n^{(n)}(x_n^\delta - x_0) \right) \tag{4.23}$$

with g_n^l given by (4.20).

We assume that the initial error satisfies the *logarithmic source condition*

$$x_0 - x^\dagger = f_p(F'[x^\dagger]^* F'[x^\dagger])w, \qquad \|w\| \le \rho, \tag{4.24a}$$

and that F is scaled such that

$$\|F'[x^\dagger]\|^2 \le \exp(-1). \tag{4.24b}$$

The total error $e_n := x_n^\delta - x^\dagger$ for Bakushinskii iterations (4.14) can be decomposed into

$$e_{n+1} = r_n\left(S_n^{(n)}\right) e_0 + g_n\left(S_n^{(n)}\right) A_n^{(n)*}\left(y^\delta - F^{(n)}(x_n^\delta) + A_n^{(n)} e_n\right)$$

with $r_n(\lambda) := 1 - \lambda g_n(\lambda)$ and $S_n^{(n)} := A_n^{(n)*} A_n^{(n)}$. Analogously, we use $S_\dagger^{(n)} := A_\dagger^{(n)*} A_\dagger^{(n)}$ with $A_\dagger^{(n)} := A_{x^\dagger}^{(n)}$. From this identity and (4.24a) it follows easily that $e_{n+1} = e_n^{\mathrm{app}} + e_n^{\mathrm{noi}} + e_n^{\mathrm{tay}} + e_n^{\mathrm{opap}} + e_n^{\mathrm{nl}}$ with

$$\begin{aligned}
e_{n+1}^{\mathrm{app}} &:= r_n(S_\dagger^{(n)}) f_p(S_\dagger^{(n)}) w,\\
e_{n+1}^{\mathrm{noi}} &:= g_n(S_n^{(n)}) A_n^{(n)*}(y^\delta - y),\\
e_{n+1}^{\mathrm{tay}} &:= g_n(S_n^{(n)}) A_n^{(n)*}\left(\int_0^1 \left(A_n^{(n)} - A_{x^\dagger + te_n}^{(n)}\right) e_n \,\mathrm{d}t\right),\\
e_{n+1}^{\mathrm{opap}} &:= r_n(S_n^{(n)})\left(f_p(S_\dagger) - f_p(S_\dagger^{(n)})\right) w + \\
&\quad + g_n(S_n^{(n)}) A_n^{(n)*}\left(y - F^{(n)}(x^\dagger) + \int_0^1 \left(A_{x^\dagger + te_n}^{(n)} - F^{(n)\prime}[x^\dagger + te_n]\right) e_n \,\mathrm{d}t\right),\\
e_{n+1}^{\mathrm{nl}} &:= \left(r_n(S_n^{(n)}) - r_n(S_\dagger^{(n)})\right) f_p(S_\dagger^{(n)}) w.
\end{aligned}$$

Here e_n^{app} is the linear approximation error, e_n^{noi} is the propagated data noise error, e_n^{tay} involves the Taylor remainder, e_n^{opap} describes the effects of the operator approximations, and e_n^{nl} the nonlinearity effect that $A_n^{(n)} \neq A_\dagger^{(n)}$ in general.

Lemma 4.6. *Assume that g_n is given by (4.20) and that for all $\bar{x}, x \in B(x^\dagger, E) = \{x : \|x - x^\dagger\| \le E\}$ there exist linear operators $R^{(n)}(\bar{x}, x) \in L(Y, Y)$ and $Q^{(n)}(\bar{x}, x) \in L(X, Y)$ such that*

$$\begin{aligned}
&A_{\bar{x}}^{(n)} = R^{(n)}(\bar{x}, x) A_x^{(n)} + Q^{(n)}(\bar{x}, x)\\
&\|I - R^{(n)}(\bar{x}, x)\| \le C_R, \quad \|Q^{(n)}(\bar{x}, x)\| \le C_Q \|A_\dagger^{(n)}(\bar{x} - x)\|
\end{aligned} \tag{4.25}$$

for all $x, \bar{x} \in B(x^\dagger, E)$ and that $\|e_n\| \le E$. Then the following estimates hold for the error components defined above

$$\|e_{n+1}^{\mathrm{app}}\| \le c_1 f_p(\alpha_n)\rho \tag{4.26a}$$

$$\|e_{n+1}^{\mathrm{noi}}\| \le \sqrt{\frac{l}{\alpha_n}}\delta \tag{4.26b}$$

$$\|e_{n+1}^{\mathrm{opap}}\| \le 2f_p(h_n)\rho + \sqrt{\frac{l}{\alpha_n}}\big(f_p(h_n) + \|e_n\|\big)h_n \tag{4.26c}$$

$$\|e_{n+1}^{\mathrm{tay}}\| \le \sqrt{\frac{l}{\alpha_n}}\left(2C_R + \frac{3}{2}EC_Q\right)\|A_\dagger^{(n)} e_n\| \tag{4.26d}$$

$$\|e_{n+1}^{\mathrm{nl}}\| \le 2^l\left((C_R+1)c_2 + \left(\frac{c_1}{2} + c_2\right)C_Q\frac{\|A_\dagger^{(n)} e_n\|}{\sqrt{\alpha_n}}\right) f_p(\alpha_n)\rho \tag{4.26e}$$

and for their images under $A_\dagger^{(n)}$

$$\|A_\dagger^{(n)} e_{n+1}^{\mathrm{app}}\| \le c_2\sqrt{\alpha_n} f_p(\alpha_n)\rho \tag{4.27a}$$

$$\|A_\dagger^{(n)} e_{n+1}^{\mathrm{noi}}\| \le \left(C_R + 1 + C_Q\|A_\dagger e_n\|\sqrt{\frac{l}{\alpha_n}}\right)\delta \tag{4.27b}$$

$$\begin{aligned}\|A_\dagger^{(n)} e_{n+1}^{\mathrm{opap}}\| \le &\left(\frac{1+C_R}{2}\sqrt{\alpha_n} + C_Q\|A_\dagger^{(n)} e_n\|\right)2f_p(h_n) + \\ &+\left(C_R + 1 + C_Q\|A_\dagger^{(n)} e_n\|\sqrt{\frac{l}{\alpha_n}}\right)\big(f_p(h_n) + \|e_n\|\big)h_n\end{aligned} \tag{4.27c}$$

$$\begin{aligned}\|A_\dagger^{(n)} e_{n+1}^{\mathrm{tay}}\| \le &\left(C_R + 1 + C_Q\|A_\dagger^{(n)} e_n\|\sqrt{\frac{l}{\alpha_n}}\right)\cdot \\ &\cdot\left(2C_R + \frac{3}{2}EC_Q\right)\|A_\dagger^{(n)} e_n\|\end{aligned} \tag{4.27d}$$

$$\begin{aligned}\|A_\dagger^{(n)} e_{n+1}^{\mathrm{nl}}\| \le 2^l &\left((C_R+1)\sqrt{\alpha_n} + C_Q\|A_\dagger^{(n)} e_n\|\right)\cdot \\ &\cdot\left((C_R+1)c_2 + (\frac{c_1}{2} + c_2)C_Q\frac{\|A_\dagger^{(n)} e_n\|}{\sqrt{\alpha_n}}\right)f_p(\alpha_n)\rho.\end{aligned} \tag{4.27e}$$

Proof. • (4.26a) and (4.27a) follow from Proposition 3.12.

• (4.26b) is a consequence of the following inequality (cf. (3.15)):

$$\|g_n^l(S_n^{(n)})A_n^{(n)*}\| \le \sqrt{\frac{l}{\alpha_n}} \tag{4.28}$$

• (4.26c) follows from Lemma 3.19, $\|r_n^l\|_\infty = 1$, the assumptions (4.22), and (4.28).

• (4.26d): By virtue of assumption (4.25) we have

$$\begin{aligned}
&\left\| \int_0^1 \left(A_n^{(n)} - A_{x^\dagger + te_n}^{(n)} \right) e_n \,\mathrm{d}t \right\| \\
\leq\ & \int_0^1 \|\big(R^{(n)}(x_n^\delta, x^\dagger) - R^{(n)}(x^\dagger + te_n, x^\dagger)\big) A_\dagger^{(n)} e_n\| \,\mathrm{d}t \\
&\qquad + \int_0^1 \|\big(Q^{(n)}(x_n^\delta, x^\dagger) - Q^{(n)}(x^\dagger + te_n, x^\dagger)\big) e_n\| \,\mathrm{d}t \\
\leq\ & \left(2C_R + \frac{3}{2} C_Q \|e_n\| \right) \|A_\dagger^{(n)} e_n\|.
\end{aligned}$$

This and (4.28) imply (4.26d).

• (4.26e): We use the decomposition

$$\begin{aligned}
&r_n^l(S_n^{(n)}) - r_n^l(S_\dagger^{(n)}) \\
=\ & \alpha_n^l (S_n^{(n)} + \alpha_n I)^{-l} \left((S_\dagger^{(n)} + \alpha_n I)^l - (S_n^{(n)} + \alpha_n I)^l \right) (S_\dagger^{(n)} + \alpha_n I)^{-l} \\
=\ & \sum_{j=0}^{l} \binom{l}{j} \left\{ \alpha_n^l (S_n^{(n)} + \alpha_n I)^{-l} \alpha_n^{l-j} \left((S_\dagger^{(n)})^j - (S_n^{(n)})^j \right) (S_\dagger^{(n)} + \alpha_n I)^{-l} \right\}.
\end{aligned}$$

Due to (4.25), the identity

$$\begin{aligned}
&(S_\dagger^{(n)})^j - (S_n^{(n)})^j \\
=\ & A_n^{(n)*} \left\{ R^{(n)}(x^\dagger, x_n^\delta)^* \big(A_\dagger^{(n)} A_\dagger^{(n)*} \big)^{j-1} - \big(A_n^{(n)} A_n^{(n)*} \big)^{j-1} R^{(n)}(x_n^\delta, x^\dagger) \right\} A_\dagger^{(n)} \\
& + Q^{(n)}(x^\dagger, x_n^\delta)^* A_\dagger^{(n)} (S_\dagger^{(n)})^{j-1} - (S_n^{(n)})^{j-1} A_n^{(n)} Q^{(n)}(x_n^\delta, x^\dagger)
\end{aligned}$$

holds for $j \geq 1$. Together with Proposition 3.12, the elementary estimate

$$\|(S_n^{(n)} + \alpha_n I)^{-1} A_n^{(n)*}\| \leq \frac{1}{2\sqrt{\alpha_n}}, \tag{4.29}$$

and (4.25) this yields

$$\begin{aligned}
&\|\alpha_n^l (S_n^{(n)} + \alpha_n I)^{-l} \alpha_n^{l-j} \left((S_\dagger^{(n)})^j - (S_n^{(n)})^j \right) (S_\dagger^{(n)} + \alpha_n I)^{-l} f_p(S_\dagger^{(n)}) w\| \\
\leq\ & \left((C_R + 1) c_2 + \left(\frac{c_1}{2} + c_2 \right) C_Q \frac{\|A_\dagger^{(n)} e_n\|}{\sqrt{\alpha_n}} \right) f_p(\alpha_n) \rho.
\end{aligned}$$

As $\sum_{j=0}^{l} \begin{pmatrix} l \\ j \end{pmatrix} = 2^l$, this gives (4.26e).

- (4.27b), (4.27d): Due to (4.25) and (4.28) we have

$$\|A_\dagger^{(n)} g_n^l(S_n^{(n)}) A_n^{(n)*}\| \le C_R + 1 + C_Q \|A_\dagger^{(n)} e_n\| \sqrt{\frac{l}{\alpha_n}}. \tag{4.30}$$

With this inequality, (4.27b) and (4.27d) can be derived just as (4.26b) and (4.26d).

- (4.27c) follows from Lemma 3.19, (4.25), and (4.29) and (4.30).

- (4.27e): With the decomposition from (4.26e), (4.27e) follows from the estimate

$$\begin{aligned} & \Big\| \big(R^{(n)}(x^\dagger, x_n^\delta) A_n^{(n)} + Q^{(n)}(x^\dagger, x_n^\delta)\big) \times \\ & \times \alpha_n^l (S_n^{(n)} + \alpha_n I)^{-l} \alpha_n^{l-j} \Big((S_\dagger^{(n)})^j - (S_n^{(n)})^j \Big) (S_\dagger^{(n)} + \alpha_n I)^{-l} f_p(S_\dagger^{(n)}) w \Big\| \\ \le \ & \Big((C_R + 1)\sqrt{\alpha_n} + C_Q \|A_\dagger^{(n)} e_n\| \Big) \times \\ & \times \left((C_R + 1) c_2 + \left(\frac{c_1}{2} + c_2\right) C_Q \frac{\|A_\dagger^{(n)} e_n\|}{\sqrt{\alpha_n}} \right) f_p(\alpha_n) \rho. \end{aligned}$$

■

For other choices of g_n in (4.14) the main difficulty is to prove estimates corresponding to (4.26e) and (4.27e).

Theorem 4.7. *Let (4.1), (4.2), (4.22), (4.24), and (4.25) hold with*

$$h_n \le \frac{1}{2} \sqrt{\frac{\alpha_n}{l}} \tag{4.31}$$

and C_R, C_Q, γ and ρ sufficiently small, and let $\alpha_0 = \exp(-1)$. Then the Gauß-Newton iterates x_n^δ, $0 \le n \le N$ given by (4.15) and (4.23) together with the stopping rule

$$\eta \alpha_{N+1} < \delta \le \eta \alpha_N \tag{4.32}$$

where η is a sufficiently small constant, are well defined and satisfy the error estimate

$$\|x_n^\delta - x^\dagger\| \le E f_p(\alpha_n), \qquad 0 \le n \le N. \tag{4.33}$$

If $\delta = 0$, we set $N = \infty$, and (4.33) holds for all $n \in \mathbb{N}$. Conditions specifying "sufficiently small" are given in the proof.

Proof. We will use an induction argument to prove the estimates

$$\theta_n \leq C_\theta \quad \text{and} \tag{4.34a}$$

$$\|e_n\| \leq C(p,n)E \tag{4.34b}$$

for $0 \leq n \leq N$ with $\theta_n := \frac{\|A_\dagger^{(n)} e_n\|}{f_p(\alpha_n)\sqrt{\alpha_n}}$ and

$$C(p,n) := 2^{-n} + \sum_{j=0}^{n-1} 2^{j-n} f_p(\alpha_j)$$

under certain smallness assumptions. We have $C(p,n) \leq 1$ since $f_p(\alpha_n) \leq 1$ and $\limsup_{n\to\infty} \frac{C(p,n)}{f_p(\alpha_n)} = 2$ since for every $q > 1$ there exists an $N \in \mathbb{N}$ such that $f_p(\alpha_j) \leq q^{n-j} f_p(\alpha_n)$ for all $n \geq N$ and $j \leq n-1$, so (4.34b) implies the assertion.

To define C_θ and to formulate the smallness assumptions we need some preparations. First note that (4.31) implies the (crude) estimate

$$f_p(h_n) \leq 2^p f_p(\alpha_n) \tag{4.35}$$

and that

$$\delta \leq \eta\gamma_p\sqrt{\alpha_n} f_p(\alpha_n) \qquad \text{with} \qquad \gamma_p := \sup_{0\leq\beta\leq\exp(-1)} \frac{\sqrt{\beta}}{f_p(\beta)} < \infty$$

for $0 \leq n \leq N$ due to (4.32). (Actually, one could choose any power α_n^ν with $\frac{1}{2} < \nu \leq 1$ in (4.32).) Moreover, (4.34b) implies $\|e_n\| \leq EC_p f_p(\alpha_n)$ with $C_p := \frac{C(p,n)}{f_p(\alpha_n)} < \infty$. Hence, if (4.34b) is true for some n, the sum of the estimates (4.27) yields the inequality

$$\|A_\dagger^{(n)} e_{n+1}\| \leq \tilde{a}\sqrt{\alpha_n} f_p(\alpha_n) + \tilde{b}\|A_\dagger^{(n)} e_n\| + \frac{\tilde{c}}{\sqrt{\alpha_n}}\|A_\dagger^{(n)} e_n\|^2$$

with constants

$$\begin{aligned}
\tilde{a} &:= c_2\rho + (C_R+1)\gamma_p\eta + +(C_R+1)2^p \\
&\quad +(C_R+1)(2^p + EC_p)\frac{1}{2\sqrt{l}} + 2^l(C_R+1)^2 c_2\rho, \\
\tilde{b} &:= C_Q\sqrt{l}\gamma_p\eta + 2^{p+1}C_Q + \frac{C_Q}{2}(2^p + EC_p) + \\
&\quad +(C_R+1)\left(2C_R + \frac{3}{2}EC_Q\right) + 2^l(C_R+1)(\frac{c_1}{2} + 2c_2)C_Q\rho, \\
\tilde{c} &:= \sqrt{l}C_Q\left(2C_R + \frac{3}{2}EC_Q\right) + 2^l C_Q^2\left(\frac{c_1}{2} + c_2\right)\rho.
\end{aligned}$$

Since $\frac{f_p(\alpha_n)}{f_p(\alpha_{n+1})} \leq C_p$ and since $f_p(\alpha_n) \leq 1$, the recursive estimate

$$\theta_{n+1} \leq a + b\theta_n + c\theta_n^2 \tag{4.36}$$

with $a := \sqrt{\gamma}C_p\left(\sqrt{E/l}+\tilde{a}\right)$, $b := \sqrt{\gamma}C_p\tilde{b}$, and $c := \sqrt{\gamma}C_p\tilde{b}$ follows from (4.22b) and (4.31).

Let t_1 and t_2 be the solutions to $a + bt + ct^2 = t$, i.e.

$$t_1 := \frac{2a}{1-b+\sqrt{(1-b)^2-4ac}}, \qquad t_2 := \frac{1-b+\sqrt{(1-b)^2-4ac}}{2c}.$$

We set $C_\theta := \max(\theta_0, t_1)$. Before we start with the induction proof, note that the sum of the estimates (4.26) together with (4.31), (4.35) and (4.34a) yields

$$\begin{aligned} \|e_{n+1}\| &\leq \frac{1}{2}\|e_n\| + C_e f_p(\alpha_n) \qquad \text{with} \\ C_e &:= c_1\rho + \eta\sqrt{l}\gamma_p + 2^{p+1}\rho + \left(2C_R + \frac{3}{2}C_Q E\right)\sqrt{l}C_\theta \\ &\quad +2^{p-1}\rho + 2^l(C_R+1)c_2\rho + 2^l\left(\frac{c_1}{2}+c_2\right)C_Q C_\theta \rho. \end{aligned} \tag{4.37}$$

We now prove (4.34) for $0 \leq n \leq N$ under the following closeness conditions:

$$b + 2\sqrt{ac} < 1 \tag{A}$$

$$\theta_0 \leq t_2 \tag{B}$$

$$C_e \leq \frac{E}{2}. \tag{C}$$

For $n = 0$, (4.34a) is true by the definition of C_θ, and (4.34b) by virtue of assumption (C) and (4.24a) since $\|e_0\| \leq \rho < C_e \leq \frac{E}{2}$. Assume that (4.34) is true for $n = k$, $k < N$. Then the assumptions of Lemma 4.6 are satisfied, and therefore (4.36) is true for $n = k$. By virtue of assumption (A) we have $t_1, t_2 \in \mathbb{R}$ and $t_1 < t_2$. By the induction hypothesis (4.34a) either $0 \leq \theta_k \leq t_1$ or $t_1 < \theta_k \leq \theta_0$ hold. In the first case, the non-negativity of a, b and c implies

$$\theta_{k+1} \leq a + b\theta_k + c\theta_k^2 \leq a + bt_1 + ct_1^2 = t_1,$$

and in the second case we use assumption (B) and the fact the $a + (b-1)t + ct^2 \leq 0$ for $t_1 \leq t \leq t_2$ to show that

$$\theta_{k+1} \leq a + b\theta_k + c\theta_k^2 \leq \theta_k \leq \theta_0.$$

Thus, in both cases (4.34a) is true for $n = k+1$. (4.34b) for $n = k+1$ follows from assumption (4.34b) and (4.37) for $n = k$ and assumption (C). ∎

We used the assumption $\alpha_0 = \exp(-1)$ in the previous theorem mainly to avoid some technical difficulties. It could easily be replaced by the assumption that α_0 is sufficiently large. For hints how to choose α_0 in practice we refer to p. 120.

Corollary 4.8. *Under the assumptions of Theorem 4.7 the order optimal convergence rate*

$$\|x_N^\delta - x^\dagger\| \leq E f_p\left(\frac{\gamma}{\eta}\delta\right) \tag{4.38}$$

holds true.

Proof. (4.15) and (4.32) imply that $\eta\frac{\alpha_N}{\gamma} \leq \eta\alpha_{N+1} < \delta$. Now the assertion follows from (4.33) and the monotonicity of f_p. ■

4.3. A convergence theorem for the discrepancy principle

Theorem 4.9. *Let (4.1), (4.2), (4.15), (4.18), and (4.24) hold with $h_n = 0$ and C_R, C_Q, r and ρ sufficiently small. Then the Gauß-Newton iterates x_n^δ given by (4.23) with $l = 1$ are well defined for $0 \leq n \leq N$ if the stopping index $N = N(\delta, y^\delta)$ is determined by the discrepancy principle*

$$\|F(x_N) - y^\delta\| \leq \tau\delta < \|F(x_n^\delta) - y^\delta\|, \qquad 0 \leq n < N \tag{4.39}$$

with a sufficiently large constant τ. The final iterates x_N^δ satisfy the order optimal estimate

$$\|x_N^\delta - x^\dagger\| = \mathrm{O}\left(f_p(\delta)\right), \qquad \delta \to 0. \tag{4.40}$$

If the α_n are chosen according to (4.16), then $N = \mathrm{O}\left(-\ln\delta\right)$.

Proof. 1.) Due to our assumptions $h_n = 0$ and $l = 1$, we have $e_n^{\mathrm{opapp}} = 0$, and the estimates (4.26e) and (4.27e) can be improved to

$$\begin{aligned}
\|e_n^{\mathrm{nl}}\| &\leq 2C_R\|A_\dagger e_{n+1}^{\mathrm{app}}\| + \left(\frac{c_1}{2} + c_2\right) C_Q \frac{\|A_\dagger e_n\|}{\sqrt{\alpha_n}} f_p(\alpha_n)\rho, \\
\|A_\dagger e_n^{\mathrm{nl}}\| &\leq \left((C_R + 1)\sqrt{\alpha_n} + C_Q\|A_\dagger e_n\|\right) \cdot \\
&\quad \cdot \left(2C_R\|A_\dagger e_{n+1}^{\mathrm{app}}\| + \left(\frac{c_1}{2} + c_2\right) C_Q \frac{\|A_\dagger e_n\|}{\sqrt{\alpha_n}} f_p(\alpha_n)\rho\right).
\end{aligned}$$

From (4.18) and (4.39) we obtain

$$\begin{aligned}
\tau\delta &\leq \|F(x_n^\delta) - F(x^\dagger) + y - y^\delta\| \\
&\leq \left\| \int_0^1 F'[x^\dagger + te_n]e_n \,\mathrm{d}t \right\| + \delta \\
&= \left\| \int_0^1 \Big(R(x^\dagger + te_n, x^\dagger) F'[x^\dagger] + Q(x^\dagger + te_n, x^\dagger) \Big) e_n \,\mathrm{d}t \right\| + \delta \\
&\leq \left(1 + C_R + \frac{1}{2}\|e_n\| C_Q\right) \|A_\dagger e_n\| + \delta,
\end{aligned}$$

and thus

$$\delta \leq \frac{1}{\tau - 1} \left(1 + C_R + \frac{1}{2}\|e_n\| C_Q\right) \|A_\dagger e_n\| \tag{4.41}$$

for $0 \leq n < N$. This gives the estimates

$$\|e_{n+1}\| \leq \left((c_1 + C_R c_2)\,\rho + \frac{cC_\theta}{C_Q} \right) f_p(\alpha_n) \tag{4.42}$$

$$\|A_\dagger e_{n+1}\| \leq \bar{a}\|A_\dagger e_{n+1}^{\mathrm{app}}\| + \tilde{b}\|A_\dagger e_n\| + \frac{\tilde{c}}{\sqrt{\alpha_n}}\|A_\dagger e_n\|^2 \tag{4.43}$$

$$\|A_\dagger e_{n+1}\| \geq \underline{a}\|A_\dagger e_{n+1}^{\mathrm{app}}\| - \tilde{b}\|A_\dagger e_n\| - \frac{\tilde{c}}{\sqrt{\alpha_n}}\|A_\dagger e_n\|^2 \tag{4.44}$$

with constants

$$\begin{aligned}
\bar{a} &:= 1 + (C_R + 1)2C_R, \qquad \underline{a} := 1 - (C_R + 1)2C_R \\
\tilde{b} &:= C_Q \left((C_R + 1)\left(c_1 + \frac{c_2}{2}\right) + C_R c_2 \right) \rho \\
&\quad + \Big(C_R + 1\Big) \left(2C_R + \frac{3}{2} C_Q E + \frac{1 + C_R + \frac{E}{2} C_Q}{\tau - 1} \right), \\
\tilde{c} &:= C_Q \left(C_Q \left(\frac{c_1}{2} + c_2 \right) \rho + 2C_R + \frac{3}{2} C_Q E + \frac{1 + C_R + \frac{E}{2} C_Q}{\tau - 1} \right).
\end{aligned}$$

provided $\|e_n\| \leq E$ and $\theta_n = \frac{\|A_\dagger e_n\|}{\sqrt{\alpha_n} f_p(\alpha_n)} \leq C_\theta$. We have the recursive estimate

$$\theta_{n+1} \leq a + b\,\theta_n + c\,\theta_n^2$$

with constants $a := \sqrt{\gamma} C_p c_2 \rho$, $b := \sqrt{\gamma} C_p \tilde{b}$, and $c := \sqrt{\gamma} C_p \tilde{c}$. If the constants s, t_1, t_2, and C_θ are defined as in the proof of Theorem 4.7, a similar induction argument shows that

$$\theta_n \leq C_\theta \qquad \text{and} \qquad \|e_n\| \leq E f_p(\alpha_n) \tag{4.45}$$

for $0 \le n \le N$ provided that

$$b + 2\sqrt{ac} < 1, \tag{A}$$

$$\theta_0 \le t_2, \tag{B}$$

$$(c_1 + C_R c_2)\,\rho + \frac{cC_\theta}{C_Q} \le \frac{E}{C_p}. \tag{C}$$

It follows from (4.41) and (4.45) that $\delta \le C\alpha_{N-1}$. This gives the estimate on N.

2.) In order to prove the convergence rate (4.40), in view of the second statement in (4.45), we only have to show that $\alpha_N = \mathrm{O}(\delta)$. By (4.43) and the first part of (4.45)

$$\|A_\dagger e_{n+1}\| \le \bar{a}\|A_\dagger e_{n+1}^{\mathrm{app}}\| + (b + cC_\Theta)\|A_\dagger e_n\|$$

holds for $0 \le n < N$. Since (C) implies $cC_\Theta \le C_Q E$, defining $q := b + C_Q E$, it follows by induction that

$$\|A_\dagger e_{n+1}\| \le \bar{a}\sum_{k=0}^{n} \|A_\dagger e_{k+1}^{\mathrm{app}}\|\, q^{n-k} + \|A_\dagger e_0\|\, q^{n+1}.$$

By spectral theory, the inequality $\lambda|r_k(\lambda)|^2 \le \gamma^2\lambda|r_{k+1}(\lambda)|^2$ for $\lambda \ge 0$ implies that

$$\|A_\dagger e_{k+1}^{\mathrm{app}}\| \le \gamma\|A_\dagger e_{k+2}^{\mathrm{app}}\|, \tag{4.46}$$

and $\lambda \le \left(\frac{\alpha_n + \|A_\dagger\|^2}{\alpha_n}\right)^2 \lambda|r_n(\lambda)|^2 \le \left(1 + \frac{\|A_\dagger\|^2}{\alpha_0}\right)^2 \gamma^n\lambda|r_n(\lambda)|^2$ for $0 \le \lambda \le \|A_\dagger\|^2$ implies that

$$\|A_\dagger e_0\| \le \left(1 + \frac{\|A_\dagger\|^2}{\alpha_0}\right)\gamma^n\|A_\dagger e_{n+1}^{\mathrm{app}}\|.$$

Hence, under the additional assumption

$$q\gamma < 1 \tag{D}$$

we obtain from the last three inequalities that

$$\|A_\dagger e_{n+1}\| \le \left(\frac{\bar{a}}{1 - q\gamma} + q\left(1 + \frac{\|A_\dagger\|^2}{\alpha_0}\right)\right)\|A_\dagger e_{n+1}^{\mathrm{app}}\|.$$

Now it follows from the lower estimate (4.44), assumption (C), $\bar{a} + \underline{a} = 2$, (4.46) and the last inequality for $n = N - 2$ that

$$\begin{aligned} \|A_\dagger e_N\| &\geq \underline{a}\|A_\dagger e_N^{\text{app}}\| - q\|A_\dagger e_{N-1}\| \\ &\geq \left(\underline{a} - \frac{q\gamma\bar{a}}{1-q\gamma} - \gamma q^2\left(1 + \frac{\|A_\dagger\|^2}{\alpha_0}\right)\right)\|A_\dagger e_N^{\text{app}}\| \\ &= \left(2 - \frac{\bar{a}}{1-q\gamma} - \gamma q^2\left(1 + \frac{\|A_\dagger\|^2}{\alpha_0}\right)\right)\|A_\dagger e_N^{\text{app}}\|. \end{aligned}$$

Furthermore, the inequality $|r_{N-1}(\lambda)|^2\lambda \geq \left(\frac{\alpha_{N-1}}{\|A_\dagger\|^2+\alpha_0}\right)^2\lambda$ implies

$$\|A_\dagger e_N^{\text{app}}\| \geq \frac{\alpha_{N-1}}{\|A_\dagger\|^2 + \alpha_0}\|A_\dagger e_0\|.$$

Using (4.18) and (4.39) we get

$$\begin{aligned} \tau\delta &\geq \|F(x_N^\delta) - F(x^\dagger) + y - y^\delta\| \\ &\geq \left\|\int_0^1 F'[x^\dagger + te_N]e_N \,\mathrm{d}t\right\| - \delta \\ &= \left\|\int_0^1 \Big(R(x^\dagger + te_N, x^\dagger)F'[x^\dagger] + Q(x^\dagger + te_N, x^\dagger)\Big)e_N \,\mathrm{d}t\right\| - \delta \\ &\geq \left(1 - C_R - \frac{1}{2}\|e_N\|C_Q\right)\|A_\dagger e_N\| - \delta, \end{aligned}$$

and thus

$$\delta \geq \frac{1}{\tau+1}\left(1 - C_R - \frac{E}{2}C_Q\right)\|A_\dagger e_N\|.$$

It follows from (D) that $1 > q > C_R + \frac{E}{2}C_Q$. Thus, putting these estimates together and imposing the additional assumption

$$\frac{\bar{a}}{1-q\gamma} + q\left(1 + \frac{\|A_\dagger\|^2}{\alpha_0}\right) < 2 \tag{E}$$

we obtain the desired estimate

$$\delta \geq C\|A_\dagger e_0\|\alpha_N, \tag{4.47}$$

where $C > 0$ is a constant independent of δ and y^δ. Since $x_0 - x^\dagger \in \mathcal{N}(A_\dagger)^\perp$ due to (4.24a), this together with (4.45) proves the convergence rate (4.40) under the smallness assumptions (A)-(E). ■

4.4. Applications

4.4.1. An inverse potential problem

In this section we consider the classical inverse problem to find the shape of a homogeneous mass distribution from measurements of its gravitational field. The same mathematical model describes the problem to find the shape of a heat source from measurements of the heat flux. This problem has recently been discussed in [Isa90a, Rin95, HR96].

In the simplest case, the *direct problem* is as follows: For a compact set $K \subset \Omega_R$, $\Omega_R := \{x \in \mathbb{R}^2 : |x| < R\}$, find the normal derivative $g := \frac{\partial u}{\partial \nu}\big|_{\partial\Omega_R}$ of the solution $u \in C^2(\Omega_R \backslash \partial K) \cap C^1(\overline{\Omega}_R)$ to the boundary value problem

$$\Delta u = \chi_D \quad \text{in } \Omega_R \backslash \partial K, \qquad u = 0 \quad \text{on } \partial\Omega_R, \tag{4.48}$$

where χ_K is the characteristic function of K and ν is the outer normal vector on $\partial\Omega_R$. It is well known that the unique solution to this problem is given by

$$u(x) = \int_K G(x, y)\,\mathrm{d}y, \tag{4.49}$$

where

$$G(x, y) := \frac{1}{2\pi} \ln|x - y| - \frac{1}{2\pi} \ln\left(\frac{|y|}{R}\left|x - \frac{R^2}{|y|^2}y\right|\right)$$

is Green's function of Ω_R. The *inverse problem* that we consider is to reconstruct K from measurement data of g. We mention that given the Cauchy data $v\big|_{\partial\Omega_R}$, $\frac{\partial v}{\partial \nu}\big|_{\partial\Omega_R}$ of any function v satisfying $\Delta v = \chi_K$, we can calculate $g = \frac{\partial u}{\partial \nu}\big|_{\partial\Omega_R}$ by evaluating a Dirichlet-to-Neumann map for the Laplace equation in Ω_R.

We restrict our attention to domains $K \subset \Omega_R$ that are starlike with respect to the origin. Then the admissible boundaries can be described by 2π-periodic functions q,

$$\partial K_q := \{z_q(t) : t \in \mathbb{R}\}, \qquad \text{where} \qquad z_q(t) := q(t)\begin{pmatrix}\cos t \\ \sin t\end{pmatrix}. \tag{4.50}$$

Define

$$D(F_{\mathrm{P}}) := \{q \in H^s([0, 2\pi]) : 0 < q < R\}, \qquad s > \frac{1}{2} \tag{4.51}$$

and let $F_P : H^s([0,2\pi]) \supset D(F_P) \to L^2([0,2\pi])$ be the operator that maps a function $q \in D(F_P)$ to the solution $g \circ \zeta_R$,

$$\zeta_R(t) := \begin{pmatrix} R\cos t \\ R\sin t \end{pmatrix} \tag{4.52}$$

to problem (4.48) for the domain K_q. Here $H^s([0,2\pi])$ denotes the Sobolev space of periodic functions on $[0,2\pi]$ with index s. Using polar coordinates, (4.49) and the identity $|x - \frac{R^2}{|y|^2}y|^2 = \frac{R^2}{|y|^2}|x-y|^2$, which holds for $|x| = R$, it is readily seen that $F_P(q)$ is given by

$$F_P(q)(t) = \int_{K_q} \frac{\partial G(\zeta_R(t), y)}{\partial \nu(x)}\,\mathrm{d}y = \int_0^{2\pi} \int_0^{q(s)} P(r, t-s) r \,\mathrm{d}r\,\mathrm{d}s, \tag{4.53}$$

where

$$P(r,t) := \frac{1}{2\pi R}\,\frac{R^2 - r^2}{R^2 + r^2 - 2Rr\cos t}$$

is the Poisson kernel. Thus we can restate our inverse problem as an operator equation

$$F_P(q) = g.$$

It can be shown that the operator F_P is injective (cf. [Isa90a]).

In order to derive Fréchet differentiability of F_P and to obtain characterizations of the derivatives of F_P we could use the method described in Chapter 1. However, we present a different approach which immediately leads to a characterization of $F_P'[q]^*$ and to an efficient numerical implementation of $F_P'[q]$. Moreover, we obtain differentiability not only with respect to the C^1-norm, but even with respect to the supremum norm.

Proposition 4.10. *The operator* $F_P : H^s([0,2\pi]) \supset D(F_P) \to L^2([0,2\pi])$, $s > \frac{1}{2}$, *is Fréchet-differentiable, and the derivative is given by*

$$\left(F_P'[q]h\right)(t) = \int_0^{2\pi} P(q(s), t-s) q(s) h(s)\,\mathrm{d}s. \tag{4.54}$$

Proof. We prove Fréchet-differentiability and (4.54) in the maximum norm. This implies the assertion since $\|\cdot\|_{H^s}$ is stronger than $\|\cdot\|_\infty$ for $s > \frac{1}{2}$ by Sobolev's embedding theorem and since $\|\cdot\|_\infty$ is stronger than $\|\cdot\|_{L^2}$. With $m := \min_{t\in[0,2\pi]} q(t)$ and $M := \max_{t\in[0,2\pi]} q(t)$, choose $\epsilon > 0$ such that $0 < m - \epsilon < M + \epsilon < R$. The function $(r,s) \mapsto \frac{\partial}{\partial r}(P(r,s)r)$ is bounded by a constant $C > 0$ on the compact set $[m-\epsilon, M+\epsilon] \times [0, 2\pi]$. Therefore, by (4.53), (4.54) and the mean value theorem, the estimate

$$\begin{aligned}
&|F_\mathrm{P}(q+h)(t) - F_\mathrm{P}(q)(t) - (F'_\mathrm{P}[q]h)(t)| \\
&= \left| \int_0^{2\pi} \int_{q(s)}^{q(s)+h(s)} \Big(P(r, t-s)r - P(q(s), t-s)q(s) \Big) \, \mathrm{d}r \, \mathrm{d}s \right| \\
&\leq 2\pi C \|h\|_\infty^2 .
\end{aligned}$$

holds for $\|h\|_\infty < \epsilon$ and $t \in [0, 2\pi]$. This proves the assertion. ∎

In the following we will often need the operator $N : H^s([0, 2\pi]) \to H^s(\partial K_q)$ which maps a function $h \in H^s([0, 2\pi])$ to the normal component of the perturbation field $\tilde{h}(z_q(t)) := h(t)(\cos t, \sin t)$ on ∂K_q, i.e. $Nh := \left\langle \tilde{h}, \nu \right\rangle$. An easy calculation shows that N is given by

$$(Nh)(z_q(t)) = \frac{q(t)h(t)}{|z'(t)|}. \tag{4.55}$$

Corollary 4.11. *Assume that $q \in D(F_\mathrm{P}) \cap C^2([0, 2\pi])$ and $h \in H^s([0, 2\pi])$, and let u' be the unique solution to the transmission problem*

$$\Delta u' = 0 \qquad \text{in } \Omega_R \backslash \partial K_q, \tag{4.56a}$$

$$u'\big|_{\partial \Omega_R} = 0, \tag{4.56b}$$

$$u'\big|_+ - u'\big|_- = 0, \tag{4.56c}$$

$$\frac{\partial u'}{\partial \nu}\Big|_+ - \frac{\partial u'}{\partial \nu}\Big|_- = Nh. \tag{4.56d}$$

Here $u'|_+$, $\frac{\partial u}{\partial \nu}|_+$ denote the limit and the normal derivative from the exterior, and $u'|_-$, $\frac{\partial u'}{\partial \nu}|_-$ the limit and normal derivative from the interior of K_q. Then $F'_\mathrm{P}[q]h$ is given by

$$F'_\mathrm{P}[q]h = \frac{\partial u'}{\partial \nu}\Big|_{\partial \Omega_R} \circ \zeta_R$$

where ζ_R is defined in (4.52).

Proof. Proposition 4.10 implies that

$$F'_\mathrm{P}[q]h = \frac{\partial v}{\partial \nu}\Big|_{\partial \Omega_R} \circ \zeta_R$$

with

$$v(x) := \int_{\partial K_q} G(x,y)(Nh)(y)\,\mathrm{d}s(y), \qquad x \in \Omega_R.$$

We have to check that v satisfies the conditions (4.56). Then the uniqueness of the transmission problem implies the assertion. Since $\Delta_x G(x,y) = 0$ for $x \neq y$ and $G(x,y) = 0$ for $x \in \partial\Omega_R$, v satisfies (4.56a) and (4.56b), where we use the boundedness of $G(x,y)$ and its derivatives for $|x-y| \geq \epsilon > 0$ to change the order of integration and differentiation. By the jump relations for the single layer potential (cf., e.g., [CK83]) v satisfies (4.56c) and (4.56d). (Note that the potential generated by the second term in the definition of $G(x,y)$ is continuously differentiable in Ω_R.) ∎

A straightforward argument using Holmgren's uniqueness theorem on $\partial\Omega_R$ shows that $F'_{\mathrm{P}}[q]$ is injective (cf. [HR96]).

Corollary 4.12. *The L^2-adjoint $F'_{\mathrm{P}}[q]^*_{L^2}$ of $F'_{\mathrm{P}}[q]$ is given by*

$$(F'_{\mathrm{P}}[q]^*_{L^2} g)(t) = q(t)v(z_q(t))$$

where v solves the Laplace equation $\Delta v = 0$ in Ω_R and satisfies the boundary condition $v|_{\partial\Omega_R} \circ \zeta_R = g$.

Proof. This follows from the formula

$$(F'_{\mathrm{P}}[q]^*_{L^2} g)(t) = q(t)\int_0^{2\pi} P(q(t), s-t)g(s)\,\mathrm{d}s$$

and $v(x) = \int_0^{2\pi} P(x, s-t)g(s)\,\mathrm{d}s$. ∎

The following formulae for $F_{\mathrm{P}}(q)$ and $F'_{\mathrm{P}}[q]$ can efficiently be evaluated numerically.

Corollary 4.13. *The following formulae hold:*

$$F_{\mathrm{P}}(q)(t) = \frac{1}{4\pi R}\int_0^{2\pi} q(s)^2\,\mathrm{d}s + \sum_{j=1}^{\infty} \frac{1}{\pi R^{j+1}(j+2)} \cdot \tag{4.57}$$
$$\cdot \left(\int_0^{2\pi} q(s)^{j+2} \cos js\,\mathrm{d}s \cos jt + \int_0^{2\pi} q(s)^{j+2} \sin js\,\mathrm{d}s \sin jt \right)$$

$$(F'_{\mathrm{P}}[q]h)(t) = \frac{1}{2\pi R}\int_0^{2\pi} q(s)h(s)\,\mathrm{d}s + \sum_{j=1}^{\infty} \frac{1}{\pi R^{j+1}} \cdot \tag{4.58}$$
$$\cdot \left(\int_0^{2\pi} q(s)^{j+1}h(s) \cos js\,\mathrm{d}s \cos jt + \int_0^{2\pi} q(s)^{j+1}h(s) \sin js\,\mathrm{d}s \sin jt \right).$$

Proof. $P(r,t)$ has the Fourier expansion

$$\begin{aligned}\frac{1}{2\pi R}\sum_{j\in\mathbb{Z}}\left(\frac{r}{R}\right)^{|j|}e^{ijt} &= \frac{1}{2\pi R}\left(\sum_{j=0}^{\infty}\left(\frac{r}{R}\right)^{j}e^{ijt}+\sum_{j=0}^{\infty}\left(\frac{r}{R}\right)^{j}e^{-ijt}-1\right)\\ &= \frac{1}{2\pi}\left(\frac{1}{R-re^{it}}+\frac{1}{R-re^{-it}}-\frac{1}{R}\right)\\ &= \frac{R(R-re^{-it}+R-re^{it})-(R^2+r^2-2Rr\cos t)}{2\pi R(R-re^{it})(R-re^{-it})}\\ &= P(r,t).\end{aligned}$$

with uniform convergence for $|r|\leq r_0<R$. We rearrange the terms on the right hand side to obtain

$$P(r,t-s)=\frac{1}{2\pi R}+\frac{1}{\pi R}\sum_{j=1}^{\infty}\left(\frac{r}{R}\right)^{j}\Big(\cos js\cos jt+\sin js\sin jt\Big).$$

Substituting this into (4.53) and (4.54) and using uniform convergence to change the order of integration and summation yields the assertion. ∎

Having studied the operators F_{P}, $F_{\mathrm{P}}'[q]$, and $F_{\mathrm{P}}'[q]^*$ we now turn our attention to the interpretation of logarithmic source conditions. We first show that Hölder-type sources conditions with $\nu\geq\frac{1}{2}$ are not fulfilled in general for the inverse potential problem even if $q_0-q^\dagger$ is very smooth, e.g. analytic. Assume that $\varphi\in\operatorname{ran}((F_{\mathrm{P}}'[q^\dagger]^*F_{\mathrm{P}}'[q^\dagger])^{\frac{1}{2}})$. Since $\operatorname{ran}((F_{\mathrm{P}}'[q^\dagger]^*F_{\mathrm{P}}'[q^\dagger])^{\frac{1}{2}})=\operatorname{ran}(F_{\mathrm{P}}'[q^\dagger]^*)$ (cf. [EHN96, Proposition 2.18.]), there exists $g\in L^2([0,2\pi])$ such that $F_{\mathrm{P}}^*[q^\dagger]g=\varphi$. Defining v as in Corollary 4.12, we find that $\varphi(t)=v(z_{q^\dagger}(t))\cdot q^\dagger(t)$. Hence $\varphi\in\operatorname{ran}(F_{\mathrm{P}}'[q^\dagger]^*)$ implies that the unique solution v to the interior Dirichlet problem for $K_{q^\dagger}$ with $v(z_{q^\dagger}(t))=\varphi(t)/q^\dagger(t)$ can be analytically extended to Ω_R. This, however, is an extremely strong assumption. The functions $\varphi(t):=\ln|x^*-z_{q^\dagger}(t)|\cdot q^\dagger(t)$ for example, with $x^*\in\Omega_R\backslash K_{q^\dagger}$, are analytic, but due to the singularity at x^* the functions $v(x)=\ln|x^*-x|$ cannot be analytically extended to Ω_R, and hence $\varphi\notin\operatorname{ran}((F_{\mathrm{P}}'[q^\dagger]^*F_{\mathrm{P}}'[q^\dagger])^{\frac{1}{2}})$.

In [HR96] it is shown that for all $q\in D(F_{\mathrm{P}})\cap C^2([0,2\pi])$ there exists $h\in L^2([0,2\pi])$ such that $F_{\mathrm{P}}'[q]^*_{L^2}F_{\mathrm{P}}'[q]_{L^2}h=q$. This, however, cannot serve as a source condition for the IRGNM, since $0\notin D(F_{\mathrm{P}})$ and since it can be seen from the proof that $\|h\|$ explodes as $\|q\|$ tends to 0.

Theorem 4.14. *Let $R>1$ and $q\equiv 1$. Then the operators*

$$f_p(F_{\mathrm{P}}'[q]^*F_{\mathrm{P}}'[q]):H^s\to H^{s+p}$$

are bounded and boundedly invertible for all $s,p>0$. Here $H^s:=H^s([0,2\pi])$.

Proof. For convenience, we consider the complex extension of $F'_{\mathrm{P}}[q]$. We use the norm

$$\|f\|_{H^s}^2 = \sum_{n\in\mathbb{Z}} (1+n^2)^s \left(\int_0^{2\pi} f(t) \mathrm{e}^{-\mathrm{i}nt} \, \mathrm{d}t \right)^2 ,$$

in $X = H^s$ (cf. [Kre89]). In order to meet the condition (4.24b), we choose the norm $\|f\|_Y := C_s \int_0^{2\pi} |f(t)|^2 \, \mathrm{d}t$ in Y with a sufficiently small scaling constant C_s. With respect to these norms the adjoint of $F'_{\mathrm{P}}[q]$ is given by

$$F'_{\mathrm{P}}[q]^* = C_s^2 j^* F'_{\mathrm{P}}[q]^*_{L^2} \tag{4.59}$$

where $j : H^s \hookrightarrow L^2$ is the embedding operator. We show that the functions

$$\varphi_n(t) := \frac{(1+n^2)^{-\frac{s}{2}}}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}nt} \qquad \text{and} \qquad \psi_n(t) := \frac{1}{C_s\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}nt} \tag{4.60}$$

are singular functions of $F'_{\mathrm{P}}[q]$. Obviously, the functions φ_n and ψ_n form Hilbert bases of X and Y, rsp. Corollary 4.12 implies $(F'_{\mathrm{P}}[q]^*_{L^2}\psi_n)(t) = v_n(1,t)$, where $v_n(r,t) := \frac{1}{C_s\sqrt{2\pi}} \left(\frac{r}{R}\right)^{|n|} \mathrm{e}^{\mathrm{i}nt}$ in polar coordinates. Therefore, $F'_{\mathrm{P}}[q]^*\psi_n$ is given by

$$F'_{\mathrm{P}}[q]^*\psi_n = C_s^2 j^* F'_{\mathrm{P}}[q]^*_{L^2}\psi_n = \frac{C_s^2}{R^{|n|}} j^*\psi_n = \sigma_n\varphi_n$$

with $\sigma_n := C_s \frac{(1+n^2)^{-\frac{s}{2}}}{R^{|n|}}$. The last equation follows from

$$\langle j^*\psi_m, \varphi_n \rangle_{H^s} = \langle \psi_m, j\varphi_n \rangle_{L^2} = \frac{(1+n^2)^{-\frac{s}{2}}}{C_s} \delta_{m,n}.$$

Moreover,

$$\langle F'_{\mathrm{P}}[q]\varphi_n, \psi_m \rangle_Y = \langle \varphi_n, F'_{\mathrm{P}}[q]^*\psi_m \rangle_X = \langle \varphi_n, \sigma_m\varphi_m \rangle_X = \sigma_m\delta_{n,m}$$

holds for all $m, n \in \mathbb{Z}$, so $F'_{\mathrm{P}}[q]\varphi_n = \sigma_n\psi_n$. This shows that $\{(\varphi_n, \psi_n, \sigma_n) : n \in \mathbb{Z}\}$ is a singular system of $F'_{\mathrm{P}}[q]$. Hence, the functional calculus is given by

$$f_p\Big(F'_{\mathrm{P}}[q]^* F'_{\mathrm{P}}[q]\Big)\varphi_n = f_p(\sigma_n^2)\varphi_n, \tag{4.61}$$

and

$$f_p(\sigma_n^2) = (2|n| \ln R - 2\ln C_s + s\ln(1+n^2))^{-p}.$$

Since we have chosen C_s such that $\max_{n\in\mathbb{Z}} \sigma_n^2 = \|F'_{\mathrm{P}}[q]\|^2 \le \exp(-1)$, an elementary calculation shows that there exist constants $c, C > 0$ such that

$$c\sqrt{1+n^2} \le 2|n|\ln R - 2\ln C_s + s\ln(1+n^2) \le C\sqrt{1+n^2},$$

holds for all $n \in \mathbb{Z}$, and therefore

$$C^{-p}(1+n^2)^{-\frac{p}{2}} \le f_p(\sigma_n^2) \le c^{-p}(1+n^2)^{-\frac{p}{2}}.$$

This and equation (4.61) imply

$$\|f_p\left(F'_{\mathrm{P}}[q]^*F'_{\mathrm{P}}[q]\right)\|_{H^s\to H^{s+p}} \le c^{-p},$$
$$\|f_p\left(F'_{\mathrm{P}}[q]^*F'_{\mathrm{P}}[q]\right)^{-1}\|_{H^{s+p}\to H^s} \le C^p,$$

which proves the theorem. ■

This theorem gives the following interpretation of the source condition (4.24) for the inverse potential problem with $q^\dagger$ representing the unit circle: $q_0 - q^\dagger = f_p(F'_{\mathrm{P}}[q^\dagger]^*F'_{\mathrm{P}}[q^\dagger])w$ for some $w \in H^s$ is equivalent to the fact that $q_0 - q^\dagger \in H^{s+p}$. Furthermore there are constants c, C such that $c\|w\|_{H^s} \le \|q_0 - q^\dagger\|_{H^{s+p}} \le C\|w\|_{H^s}$, i.e. smallness of $\|w\|_{H^s}$ corresponds to smallness of $\|q_0 - q^\dagger\|_{H^{s+p}}$.

4.4.2. Inverse sound-soft scattering problem

We consider the problem to reconstruct a sound-soft scatterer K from far field measurements corresponding to one incident wave as described in the introduction. Again, we assume that K is star-like with respect to the origin and that ∂K is described by a radial function q as in (4.50). We define the operator

$$F_{\mathrm{D}} : q \mapsto u_\infty$$

that maps a radial function q in

$$D(F_{\mathrm{D}}) := \{q \in H^s_{\mathbb{R}} : q > 0\}$$

to the far field pattern u_∞ in $Y = L^2_{\mathbb{C}}(S^1)$ corresponding to the scatterer K_q.

It is an open problem whether or not the operator F_{D} in this form is one-to-one. According to a result by Schiffer (cf. [CK97]) a sound-soft obstacle is uniquely determined by the far-field patterns of an infinite number of distinct incident plane waves with the same wave number. Moreover, Colton and

Sleeman ([CS83, CK97]) have shown that a sound-soft obstacle is uniquely determined by the far-field pattern for *one* incident wave and the a-priori information that the obstacle is contained in a ball of radius $R < \gamma/\kappa$ where γ is the first positive zero of the Bessel function J_0. These results do not require the information that the obstacle is star-shaped.

We have shown in Chapter 1 that the operator F_{D} is differentiable if the variations of the domain are measured by the norm $\|z_q\|_{C^1}$ (z_q given by (4.50)). Since

$$\|z_q\|_{C^1} = \|q\|_\infty + \|\sqrt{q^2 + q'^2}\|_\infty,$$

this is equivalent to differentiability with respect to the norm $\|q\|_{C^1}$. By Sobolev's embedding theorem, the norms $\|\cdot\|_{H^s}$ are stronger than $\|\cdot\|_{C^1}$ for $s > \frac{3}{2}$. Therefore, Theorem 1.12 is applicable for $s > \frac{3}{2}$, and the derivative of F_{D} is given by

$$F'_{\mathrm{D}}[q]h = -A_{\mathrm{D}} \frac{\partial u}{\partial \nu} N h. \tag{4.62}$$

Here $N : H^s_{\mathbb{R}}([0, 2\pi]) \to H^s_{\mathbb{C}}(\partial K_q)$ is defined in (4.55), and A_{D} is the solution operator for the exterior Dirichlet problem, i.e. A_{D} maps a function $f \in H^s(\partial K_q)$ to the far field pattern v_∞ of the radiating solution v of the Helmholtz equation with boundary condition $v\big|_{\partial K_q} = f$. As we have seen in Section 2.1., A_{D} is given by

$$A_{\mathrm{D}} = 2\mathcal{F}(I + D - \mathrm{i}\eta S)^{-1} \tag{4.63}$$

with the far field operator

$$\mathcal{F} f(\hat{x}) := \frac{\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}}{\sqrt{8\pi\kappa}} \int_{\partial K_q} (\langle \nu(y), -\mathrm{i}\kappa\hat{x}\rangle - \mathrm{i}\eta)\, \mathrm{e}^{-\mathrm{i}\kappa\langle \hat{x}, y\rangle} f(y)\, \mathrm{d}s(y) \tag{4.64}$$

corresponding to the mixed layer potential.

Before we characterize the adjoint of $F'[q]$, let us clarify the roles of the different dual systems of complex Hilbert spaces. Recall from p. 13 that we have to interpret complex Hilbert spaces as real Hilbert spaces since the boundaries are described by elements of real spaces.

Remark 4.15. Let X and Y be complex Hilbert spaces with a involution $^-$ and inner products $\langle\cdot,\cdot\rangle^X_{\mathbb{C}}$ and $\langle\cdot,\cdot\rangle^Y_{\mathbb{C}}$, rsp., and let $T : X \to Y$ be a linear bounded operator. Moreover, let $(f, g)^{X,Y} := \langle f, \bar{g}\rangle^{X,Y}_{\mathbb{C}}$ be the corresponding bilinear forms and $\langle f, g\rangle^{X,Y}_{\mathbb{R}} := \mathrm{Re}\,\langle f, g\rangle^{X,Y}_{\mathbb{C}}$ the inner products of X and Y as real Hilbert spaces. We denote the adjoint of T with respect to $(\cdot,\cdot)^{X,Y}$

by T', and the adjoint with respect to $\langle\cdot,\cdot\rangle_{\mathbb{C}}^{X,Y}$ by T^*. It follows immediately from these definitions that

$$T'f = \overline{T^*\bar{f}},$$

and that the adjoints with respect to $\langle\cdot,\cdot\rangle_{\mathbb{C}}^{X,Y}$ and $\langle\cdot,\cdot\rangle_{\mathbb{R}}^{X,Y}$ coincide.

The following results can be found in [Kir89a] and [HHS95]. Our approach has the advantage that there is an obvious analogous discrete version which leads to the adjoint A_n^* of the numerical approximation A_n to $F'[q_n^\delta]$ that is described in Chapter 2 (cf. also Section 5.1.). For the performance of the Newton-CG method it is advantageous to approximate $F'[q_n^\delta]^*$ by A_n^* instead of using any approximation to $F'[q_n^\delta]^*$. Modifications for limited aperture problems and near field data are obvious.

Proposition 4.16. *1. Let*

$$v_{\mathrm{i}}^g(y) := \frac{e^{\mathrm{i}\frac{\pi}{4}}}{\sqrt{8\pi\kappa}} \int_{S^1} e^{-\mathrm{i}\kappa\langle\hat{x},y\rangle} g(\hat{x})\,\mathrm{d}s(\hat{x}), \qquad y \in \mathbb{R}^2 \tag{4.65}$$

be the Herglotz wave function with kernel $g \in L^2(S^1)$. Then

$$\mathcal{F}^* g = \overline{\left(\frac{\partial v_{\mathrm{i}}^{\bar{g}}}{\partial\nu} - \mathrm{i}\eta v_{\mathrm{i}}^{\bar{g}}\right)}\Big|_{\partial K}. \tag{4.66}$$

2. Let v^g be the total field for the incident wave v_{i}^g given by (4.65), i.e. $v^g = v_s^g + v_i^g$ where $v = 0$ on ∂K, and v_s^g satisfies (0.1) and (0.4). Then the L^2-adjoint of A_{D} is given by

$$A_{\mathrm{D},L^2}^* g = \overline{\frac{\partial v^{\bar{g}}}{\partial\nu}}. \tag{4.67}$$

3.

$$F_{\mathrm{D}}'[q]_{L^2}^* g = -q \cdot \mathrm{Re}\left(\overline{\frac{\partial u}{\partial\nu}} \cdot \overline{\frac{\partial v^{\bar{g}}}{\partial\nu}}\right) \circ z_q. \tag{4.68}$$

Proof. (4.66) is an immediate consequence of the definitions. As in (2.5), $\frac{\partial v^{\bar{g}}}{\partial\nu}$ is given by

$$\frac{\partial v^{\bar{g}}}{\partial\nu} = 2(I + D' - i\eta S)\left(\frac{\partial v_{\mathrm{i}}^{\bar{g}}}{\partial\nu} - \mathrm{i}\eta v_{\mathrm{i}}^{\bar{g}}\right).$$

Due to (4.63), Remark 4.15, and (4.66) we have

$$A^*_{\mathrm{D},L^2} = 2(I + (D - \mathrm{i}\eta S)^*)^{-1}\mathcal{F}^* = \overline{2(I + D' - i\eta S)\left(\frac{\partial v_{\mathrm{i}}^{\bar{g}}}{\partial \nu} - \mathrm{i}\eta v_{\mathrm{i}}^{\bar{g}}\right)}.$$

This gives (4.67). Finally, we have

$$\langle Nh, f\rangle_{L^2_{\mathbb{C}}(\partial K_q)} = \mathrm{Re}\int_0^{2\pi} \frac{h\,q}{|z_q'|}\,\overline{f\circ z_q}\,|z_q'|\,\mathrm{d}t = \langle h, q\cdot \mathrm{Re}\, f\circ z_q\rangle_{L^2_{\mathbb{R}}([0,2\pi])}$$

for all $h \in L^2_{\mathbb{R}}([0,2\pi])$ and $f \in L^2_{\mathbb{C}}(\partial K_q)$, so $N^* f = q \cdot \mathrm{Re}\, f\circ z_q$. Hence, (4.68) follows from (4.62) and (4.67). ■

The intermediate results (4.66) and (4.67) have important consequences. It follows form (4.67) that A_{D} has dense range (cf. [Kir89a]). It can also be shown that the complex extension $F'[q]_{\mathbb{C}}$ has dense range (cf. [KR94, HHS95]), but $F'[q]$ does not.

We now use (4.66) to show that Hölder-type source conditions are extremely restrictive for the sound-soft scattering problem. Assume first that $f \in \mathrm{ran}((\mathcal{F}^*\mathcal{F})^{\frac{1}{2}}) = \mathrm{ran}(\mathcal{F}^*)$, i.e. there exists $g \in L^2_{\mathbb{C}}(S^1)$ such that $\mathcal{F}^* g = f$. Then the unique solution to the interior Robin problem in K_q with boundary condition

$$\frac{\partial w}{\partial \nu} - \mathrm{i}\eta w = \bar{f} \qquad \mathrm{on} K_q$$

coincides with $v_{\mathrm{i}}^{\bar{g}}$. Hence, w can be analytically extended to $\mathbb{R}^2$ as a Herglotz wave function. This, however, is an extremely strong condition, which is not fulfilled for the analytic functions $f(x) = \Phi(x, x^*)$ with $x^* \notin K_q$, for example. (Φ is the fundamental solution defined in (2.2)). If $q \in C^\infty([0,2\pi])$, it follows from Riesz theory and the mapping properties of the boundary integral operators (cf. [Kir89b]) that $I + D' - \mathrm{i}\eta S$ is a homeomorphism for all Sobolev spaces $H^l_{\mathbb{C}}(\partial K_q)$, and that $\frac{\partial u}{\partial \nu} \in C^\infty(\partial K_q)$ (cf. (2.5)). Therefore, the condition $f \in \mathrm{ran}(F'_{\mathrm{D}}[q]^*)$ is about as restrictive as $f \in \mathrm{ran}(\mathcal{F}^*)$.

Again, appropriate source conditions for the sound-soft scattering problem are of logarithmic type.

Theorem 4.17. *Let $r, s, p > 0$, and consider the case of a circle, i.e. $q \equiv r$. Then the inclusions*

$$H^{s+p+\epsilon}_{\mathbb{C}} \subset f_p(A^*_{\mathrm{D}}A_{\mathrm{D}})(H^s_{\mathbb{C}}) \subset H^{s+p}_{\mathbb{C}}$$

hold for all $\epsilon > 0$, and the operators

$$f_p(A^*_{\mathrm{D}}A_{\mathrm{D}}) : H^s_{\mathbb{C}} \to H^{s+p}_{\mathbb{C}},$$
$$(f_p(A^*_{\mathrm{D}}A_{\mathrm{D}}))^{-1} : H^{s+p+\epsilon}_{\mathbb{C}} \to H^s_{\mathbb{C}}$$

are bounded. Here $H^s_{\mathbb{C}} = H^s_{\mathbb{C}}(\partial K_q)$.

Proof. It follows from Remark 4.15 that the set of singular values of A_{D} is the same with respect to the real and complex inner product and that the multiplicity of the $\langle\cdot,\cdot\rangle_{\mathbb{R}}$-singular values is twice as high as that of the $\langle\cdot,\cdot\rangle_{\mathbb{C}}$-singular values. Therefore, we may interpret $H^s_{\mathbb{C}}$ and $L^2_{\mathbb{C}}(S^1)$ as complex Hilbert spaces in the usual way for this proof. Moreover, by a simple rescaling, we may assume w.l.o.g. that $r = 1$.

Let the norm in Y be given by $\|f\|^2_Y := C_s^2 \int_{S^1} |f|^2 \,\mathrm{d}s$ with a scaling constant $C_s > 0$ such that (4.24b) is satisfied. We show that the functions

$$\varphi_n\left(\begin{pmatrix}\cos t\\ \sin t\end{pmatrix}\right) := \frac{(1+n^2)^{-\frac{s}{2}}}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}nt} \quad \text{and} \quad \psi_n\left(\begin{pmatrix}\cos t\\ \sin t\end{pmatrix}\right) = \frac{1}{C_s\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}nt} \tag{4.69}$$

($n \in \mathbb{Z}$) are singular functions of $F'_{\mathrm{D}}[q]$. It is well known that $\{\varphi_n : n \in \mathbb{Z}\}$ and $\{\psi_n : n \in \mathbb{Z}\}$ are Hilbert bases of $H^s_{\mathbb{C}}(\partial K_q)$ and $L^2_{\mathbb{C}}(S^1)$, rsp. The radiating solutions v_n to the Helmholtz equation with Dirichlet boundary values φ_n are given by

$$v_n(r,t) = \frac{(1+n^2)^{-\frac{s}{2}}}{\sqrt{2\pi}} \frac{H^{(1)}_{|n|}(\kappa r)}{H^{(1)}_{|n|}(\kappa)}\mathrm{e}^{\mathrm{i}nt}$$

in polar coordinates where $H^{(1)}_m$ denotes the Hankel function of order $m \in \mathbb{N}_0$ of the first kind. From the asymptotic behavior of the Hankel functions for large arguments

$$H^{(1)}_m(t) = \sqrt{\frac{2}{\pi t}}\mathrm{e}^{\mathrm{i}(t-\frac{m\pi}{2}-\frac{\pi}{4})}\left(1 + \mathrm{O}\left(\frac{1}{t}\right)\right), \qquad t \to \infty, \tag{4.70}$$

$m \in \mathbb{N}_0$, and (0.5) it follows that the far field patterns $v_{n,\infty}$ of v_n are given by $v_{n,\infty} = \sigma_n\psi_n$, where

$$\sigma_n := C_s(1+n^2)^{-\frac{s}{2}}\frac{1}{H^{(1)}_{|n|}(\kappa)}\sqrt{\frac{2}{\pi k}}\mathrm{e}^{\mathrm{i}(-\frac{|n|\pi}{2}-\frac{\pi}{4})}.$$

Hence $\{(\varphi_n, \frac{\sigma_n}{|\sigma_n|}\psi_n, |\sigma_n|) : n \in \mathbb{Z}\}$ is a singular system of A_{D}, and $f_p(A^*_{\mathrm{D}}A_{\mathrm{D}})$ is given by

$$f_p(A^*_{\mathrm{D}}A_{\mathrm{D}})\varphi_n = f_p(|\sigma_n|^2)\varphi_n. \tag{4.71}$$

From the asymptotic formula 1.5) and from Stirling's formula

$$n! = \sqrt{2\pi n}(n/\mathrm{e})^n(1 + o(1)) \tag{4.72}$$

it can be seen that

$$|\sigma_n| = \frac{C_s}{\sqrt{\kappa}}(1+n^2)^{-\frac{s}{2}}\left(\frac{\kappa}{2}\right)^{|n|}\frac{1}{\sqrt{|n|-1}}\left(\frac{\mathrm{e}}{|n|-1}\right)^{|n|-1}(1+o(1))$$

for $|n| \to \infty$. An elementary calculation shows that for $\epsilon > 0$ there exist constants $C', C > 0$ such that for all $n \in \mathbb{Z}$

$$\begin{aligned} -\ln|\sigma_n|^2 \;\leq\; & C' + s\ln(1+n^2) - 2|n|\ln\frac{\kappa}{2} + \ln(|n|-1) + \\ & +2(|n|-1)\ln\frac{|n|-1}{\mathrm{e}} \leq C(1+n^2)^{\frac{1+\epsilon/p}{2}}. \end{aligned}$$

Furthermore there exist constants $N_0 \in \mathbb{N}$ and $c' > 0$ such that for $|n| > N_0$

$$-\ln|\sigma_n|^2 \geq c'\sqrt{1+n^2}$$

holds. Since we have chosen C_s such that $-\ln|\sigma_n|^2 \geq 1$ for all $n \in \mathbb{Z}$, setting $c := \min(c', (1+N_0^2)^{-\frac{1}{2}})$ we obtain

$$-\ln|\sigma_n|^2 \geq c\sqrt{1+n^2} \qquad \text{for } n \in \mathbb{Z}.$$

From these estimates it follows that

$$C^{-p}(1+n^2)^{-\frac{p+\epsilon}{2}} \leq f_p(|\sigma_n|^2) \leq c^{-p}(1+n^2)^{-\frac{p}{2}} \tag{4.73}$$

for $n \in \mathbb{Z}$. The second inequality together with 4.71 implies that $f_p(A_{\mathrm{D}}^* A_{\mathrm{D}})$ maps $H^s_{\mathbb{C}}$ boundedly into $H^{s+p}_{\mathbb{C}}$. The first inequality implies that $H^{s+p+\epsilon}_{\mathbb{C}} \subset f_p(A_{\mathrm{D}}^* A_{\mathrm{D}})(H^s_{\mathbb{C}})$ and that $(f_p(A_{\mathrm{D}}^* A_{\mathrm{D}}))^{-1} : H^{s+p+\epsilon}_{\mathbb{C}} \to H^s_{\mathbb{C}}$ is bounded. ■

Remark 4.18. The result of the previous theorem is simpler if we consider the problem to reconstruct ∂K from *near field data* $u_s\big|_{\{|x|=R\}}$ instead of the far field data u_∞. Let $\tilde{A_{\mathrm{D}}}$ be the operator that maps a function f to $v\big|_{\{|x|=R\}}$ where v is the radiating solution to the Helmholtz equation with boundary values $v|_{\partial K_q} = f$. We assume that $R > 0$ is sufficiently large such that $K \subset B_R(0)$. Then, under the assumptions of Theorem 4.17, we have

$$H^{s+p}_{\mathbb{C}} = f_p(\tilde{A_{\mathrm{D}}}^*\tilde{A_{\mathrm{D}}})(H^s_{\mathbb{C}}),$$

and $f_p(\tilde{A_{\mathrm{D}}}^*\tilde{A_{\mathrm{D}}}) : H^s_{\mathbb{C}} \to H^{s+p}_{\mathbb{C}}$ is bounded and boundedly invertible. The proof is analogous to that of Theorem 4.17. The singular values of $\tilde{A_{\mathrm{D}}}$ are

$$\sigma_n = C_s(1+n^2)^{-\frac{s}{2}}\frac{H^{(1)}_{|n|}(R\kappa)}{H^{(1)}_{|n|}(\kappa)}$$

and have the asymptotic behavior

$$|\sigma_n| = C_s(1+n^2)^{-\frac{s}{2}} R^{-|n|}\left(1 + \mathrm{O}\left(\frac{1}{|n|}\right)\right), \qquad |n| \to \infty$$

due to (1.5).

In order to interpret the source condition (4.24) for the sound-soft scattering problem, we are actually interested in $F'_{\mathrm{D}}[q]$ for general $q \in D(F_{\mathrm{D}})$ instead of $A_{\mathrm{D},const}$. Although we do not know a singular system of $F'_{\mathrm{D}}[q]$ even for $q \equiv const$, we will show that the singular values of $F'_{\mathrm{D}}[q]$ and $A_{\mathrm{D},const}$ have the same asymptotic behavior. These estimates are based on the fact that the singular values (numbered in decreasing order with multiplicity) obey

$$\begin{aligned} \sigma_n(ABC) &\leq \|A\|\sigma_n(B)\|C\| \qquad \text{and} \\ \sigma_{2n}(B+\tilde{B}) &\leq \sigma_n(B) + \sigma_n(\tilde{B}) \end{aligned}$$

if $A: X_1 \to X_2$ and $C: X_3 \to X_4$ are bounded linear operators, and $B, \tilde{B}: X_2 \to X_3$ are compact linear operators between Hilbert spaces X_1, X_2, X_3 and X_4 (cf., e.g., [MV92]).

We first consider the operator $A_{\mathrm{D},q}$ for general $q \in D(F_{\mathrm{D}})$. If $q_1 < q_2$, $q_1, q_2 \in D(F_{\mathrm{D}})$, let $U_{q_1\to q_2} : H^s_{\mathbb{C}}(\partial K_{q_1}) \to H^s_{\mathbb{C}}(\partial K_{q_2})$ be the operator that maps a function $f \in H^s_{\mathbb{C}}(\partial K_{q_1})$ to $U_{q_1\to q_2} f := v|_{\partial K_{q_2}}$ where v is the radiating solution to the Helmholtz equation with boundary values $v = f$ on ∂K_{q_1}. It is easy to show that $U_{q_1\to q_2}$ is bounded and that $A_{\mathrm{D},q_1} = A_{\mathrm{D},q_2} U_{q_1\to q_2}$. For $q \in D(F_{\mathrm{D}})$ choose $r, R \in \mathbb{R}$ such that $0 < r < q < R$. Then

$$\begin{aligned} \sigma_n(A_{\mathrm{D},r}) &= \sigma_n(A_{\mathrm{D},q}U_{r\to q}) \leq \sigma_n(A_{\mathrm{D},q})\|U_{r\to q}\| \quad \text{and} \\ \sigma_n(A_{\mathrm{D},q}) &= \sigma_n(A_{\mathrm{D},R}U_{q\to R}) \leq \sigma_n(A_{\mathrm{D},R})\|U_{q\to R}\|, \end{aligned}$$

so

$$\frac{1}{\|U_{r\to q}\|}\sigma_n(A_{\mathrm{D},r}) \leq \sigma_n(A_{\mathrm{D},q}) \leq \|U_{q\to R}\|\sigma_n(A_{\mathrm{D},R})$$

for all $n \in \mathbb{N}$. Hence,

$$\sigma_n(f_p(A^*_{\mathrm{D},q}A_{\mathrm{D},q})) \sim \sigma_n(f_p(A^*_{\mathrm{D},r}A_{\mathrm{D},r})) \sim \sigma_n(f_p(A^*_{\mathrm{D},R}A_{\mathrm{D},R})).$$

Now we turn our attention to the operator $M := -\frac{\partial u}{\partial \nu}N : H^s_{\mathbb{R}}([0,2\pi]) \to H^s_{\mathbb{C}}(\partial K_q)$. The complex extension $M_{\mathbb{C}} : H^s_{\mathbb{C}}([0,2\pi]) \to H^s_{\mathbb{C}}(\partial K_q)$ of M is bounded and boundedly invertible if q and $\frac{\partial u}{\partial \nu}$ are s times continuously differentiable and if $\frac{\partial u}{\partial \nu}$ does not have zeros. In this case the operator $F'_{\mathrm{D}}[q]_{\mathbb{C}} := A_{\mathrm{D}}M_{\mathbb{C}}$ satisfies the estimates

$$\begin{aligned} \sigma_n(F'_{\mathrm{D}}[q]_{\mathbb{C}}) = \sigma_n(A_{\mathrm{D}}M_{\mathbb{C}}) \leq \|M_{\mathbb{C}}\|\sigma_n(A_{\mathrm{D}}), \\ \sigma_n(A_{\mathrm{D}}) = \sigma_n(F'_{\mathrm{D}}[q]_{\mathbb{C}}M_{\mathbb{C}}^{-1}) \leq \|M_{\mathbb{C}}^{-1}\|\sigma_n(F'_{\mathrm{D}}[q]_{\mathbb{C}}), \end{aligned}$$

i.e. the singular values of $F'_{\mathrm{D}}[q]_{\mathbb{C}}$ and A_{D} have the same asymptotic behavior.

From $F'_{\mathrm{D}}[q]_{\mathbb{C}} h = F'_{\mathrm{D}}[q](\mathrm{Re}\, h) + \mathrm{i} F'_{\mathrm{D}}[q](\mathrm{Im}\, h)$ we conclude that

$$\sigma_{2n}(F'_{\mathrm{D}}[q]_{\mathbb{C}}) \leq \sigma_n(F'_{\mathrm{D}}[q]) + \sigma_n(\mathrm{i}F'_{\mathrm{D}}[q]) = 2\sigma_n(F'_{\mathrm{D}}[q]).$$

Moreover, since $F'_{\mathrm{D}}[q]$ is a restriction of $F'_{\mathrm{D}}[q]_{\mathbb{C}}$, we obtain

$$\sigma_n(F'_{\mathrm{D}}[q]) \leq \sigma_n(F'_{\mathrm{D}}[q]_{\mathbb{C}}).$$

Therefore, the singular values $\sigma_n(F'_{\mathrm{D}}[q])$ also satisfy (4.73) with different constants c and C.

If q describes the unit circle, it can be seen from the representation

$$\frac{\partial u}{\partial \nu}\left(\begin{pmatrix} \cos t \\ \sin t \end{pmatrix}\right) = \frac{2}{\mathrm{i}\pi} \sum_{n\in-\infty}^{\infty} \frac{\mathrm{i}^n \mathrm{e}^{\mathrm{i}n(t-t_0)}}{H_n(\kappa)},$$

with $d = (\cos t_0, \sin t_0)^T$ and $H^{(1)}_{-n} = (-1)^n H^{(1)}_n$ (cf. [KR94]), that $M_{\mathbb{C}} : H^s_{\mathbb{C}}([0, 2\pi]) \to H^s_{\mathbb{C}}(\partial K_q)$ is indeed a homeomorphism at least for sufficiently small κ.

In summary, (4.24) with $F = F_{\mathrm{D}}$ is a closeness condition in a $(s+p+\epsilon)$-“Sobolev space” with respect to some unknown basis functions.

4.4.3. Inverse sound-hard scattering problem

In this subsection we discuss the source condition (4.24) for the sound-hard scattering problem. We define F_{N} to be the operator that maps $q \in H^s_{\mathbb{R}}([0, 2\pi])$ to the far field pattern u_∞ that corresponds to the sound-hard scatterer K_q described by (4.50).

Although it is not known if the operator F_{N} in this form is one-to-one, it has been shown by Isakov ([Isa90b], cf. also [CK97]) that a sound-hard obstacle is uniquely determined by the far-field patterns of an infinite number of distinct incident plane waves. In fact, as noted in [Kir98], these data also determine the boundary condition.

By Theorem 1.17 and the remarks in Subsection 4.4.2., F_{N} is Fréchet differentiable for $s > \frac{3}{2}$. The derivative can be written as

$$F'_{\mathrm{N}}[q]h = A_N B N \tag{4.74}$$

where N is defined in (4.55), $B : H^s_{\mathbb{R}} \to H^{s-1}_{\mathbb{C}}$ is given by

$$Bf := \frac{d}{ds}\left(f \frac{du}{ds}\right) + \kappa^2 u f,$$

and $A_{\mathrm{N}} : H^{s-1}_{\mathbb{C}}(\partial K_q) \to L^2_{\mathbb{C}}(S^1)$ maps a function $\varphi \in H^{s-1}_{\mathbb{C}}(\partial K_q)$ to the far field pattern v_∞ of the radiating solution v to the Helmholtz equation with Neumann boundary values $\frac{\partial v}{\partial \nu} = \varphi$ on ∂K_q. We have seen in Section 2.1., A_{N} can be written as

$$A_{\mathrm{N}} = 2\mathcal{F}(T - \mathrm{i}\eta D' + \mathrm{i}\eta I)^{-1}$$

with the far field operator $\mathcal{F}$ defined in (4.64).

For the following results we refer to [Kir89a] and [Het96].

Proposition 4.19. *1. Let v^g be the total field for the incident wave v^g_{i} given by (4.65), i.e. $v^g = v^g_s + v^g_i$ where $\frac{\partial v}{\partial \nu} = 0$ on ∂K and v^g_s satisfies (0.1) and (0.4). Then*

$$A^*_{\mathrm{N},L^2} g = -\overline{v^{\bar{g}}}. \tag{4.75}$$

2. The L^2-adjoint of $F'_{\mathrm{N}}[q]$ is given by

$$F'_{\mathrm{N}}[q]^* g = q \cdot \mathrm{Re}\left(\overline{\frac{\partial u}{\partial s}} \cdot \overline{\frac{dv^{\bar{g}}}{ds}} - \overline{\kappa^2 u \cdot} \cdot \overline{v^{\bar{g}}}\right) \circ z_q. \tag{4.76}$$

Proof. As in (2.7) we have

$$-v^{\bar{g}} = 2(T - \mathrm{i}\eta D + \mathrm{i}\eta I)^{-1}\left(\frac{\partial v^{\bar{g}}_{\mathrm{i}}}{\partial \nu} - \mathrm{i}\eta v^{\bar{g}}_{\mathrm{i}}\right).$$

On the other hand, using Remark 4.15, (4.66), and (4.74), we get

$$\begin{aligned} A^*_{\mathrm{N},L^2} g &= 2\left((T - \mathrm{i}\eta D + \mathrm{i}\eta I)^{-1}\right)^* \mathcal{F}^* g \\ &= \overline{2(T - \mathrm{i}\eta D' + \mathrm{i}\eta I)^{-1}\left(\frac{\partial v^{\bar{g}}_{\mathrm{i}}}{\partial \nu} - \mathrm{i}\eta v^{\bar{g}}_{\mathrm{i}}\right)}. \end{aligned}$$

This gives (4.75). Since the adjoint of the arc-length derivative $\frac{d}{ds}$ is $-\frac{d}{ds}$, the adjoint of B is given by $B^* f = -\frac{df}{ds}\frac{d\bar{u}}{ds} + \kappa^2 \bar{u} f$, and we already know from the proof of Proposition 4.16 that $N^* f = q \cdot \mathrm{Re}\, f \circ z_q$. Hence, (4.76) follows from (4.74) and (4.75). ■

Let us now turn to logarithmic source conditions.

Theorem 4.20. *Let $q \equiv r$ and $r, s, p > 0$. Then the inclusions*

$$H^{s+p+\epsilon}_{\mathbb{C}} \subset f_p(A^*_{\mathrm{N}} A_{\mathrm{N}})(H^s_{\mathbb{C}}) \subset H^{s+p}_{\mathbb{C}} \tag{4.77}$$

hold for all $\epsilon > 0$, and the operators

$$\begin{aligned} &f_p(A^*_{\mathrm{N}} A_{\mathrm{N}}) : H^s_{\mathbb{C}} \to H^{s+p}_{\mathbb{C}}, \\ &(f_p(A^*_{\mathrm{N}} A_{\mathrm{N}}))^{-1} : H^{s+p+\epsilon}_{\mathbb{C}} \to H^s_{\mathbb{C}} \end{aligned}$$

are bounded. Here $H^s_{\mathbb{C}} := H^s_{\mathbb{C}}(\partial K)$.

Proof. As in the proof of Theorem 4.17 we may interpret $H^s_{\mathbb{C}}$ and $L^2_{\mathbb{C}}(S^1)$ as complex Hilbert spaces in the usual way and assume that $r = 1$. Recall the definition of the scaling constant C_s and the Hilbert bases (4.69). The radiating solution to the Helmholtz equation satisfying the Neumann boundary condition $\frac{\partial v_n}{\partial \nu} = \varphi_n$ is

$$v_n(r,t) = \frac{(1+n^2)^{-\frac{s}{2}}}{\sqrt{2\pi}} \cdot \frac{H^{(1)}_{|n|}(\kappa r)}{\kappa H^{(1)\prime}_{|n|}(\kappa)} \mathrm{e}^{int}$$

in polar coordinates. It follows from (4.70) and (0.5) that the far field patterns $v_{n,\infty} = A_{\mathrm{N}}\varphi_n$ of v_n are given by $v_{n,\infty} = \sigma_n \psi_n$, where

$$\sigma_n := C_s \frac{(1+n^2)^{-\frac{s}{2}}}{\kappa H^{(1)\prime}_{|n|}(\kappa)} \sqrt{\frac{2}{\pi\kappa}} \mathrm{e}^{\mathrm{i}(-\frac{|n|\pi}{2} - \frac{\pi}{4})}.$$

This implies that a singular system of A_{N} is given by $\{(\varphi_n, \frac{\sigma_n}{|\sigma_n|}\psi_n, |\sigma_n|) : n \in \mathbb{Z}\}$. Hence the operator $f_p(A^*_{\mathrm{N}} A_{\mathrm{N}})$ can be written as in (4.71). The identity $H^{(1)\prime}_n(t) = H^{(1)}_{n-1}(t) - \frac{n}{t} H^{(1)}_n(t)$, $n \geq 1, t > 0$, (1.5), and (4.72) yield the asymptotic formula

$$|\sigma_n| = C_s \frac{1}{\sqrt{\kappa}} |n|^{-s-\frac{1}{2}} \left(\frac{\kappa \mathrm{e}}{2|n|}\right)^{|n|} \Big(1 + o(1)\Big), \qquad |n| \to \infty,$$

and hence

$$-\ln|\sigma_n|^2 = \left(-\ln\frac{C_s^2}{\kappa} + (2s+1)\ln|n| + 2|n|\ln\left(\frac{2|n|}{\kappa \mathrm{e}}\right)\right)\Big(1 + \mathrm{o}(1)\Big)$$

for $|n| \to \infty$. For all $\epsilon > 0$ there exist constants $c, C > 0$ and $N_0 \in \mathbb{N}$ such that

$$c\sqrt{1+n^2} \leq -\ln|\sigma_n|^2 \leq C(1+n^2)^{\frac{1+\epsilon/p}{2}} \qquad |n| \geq N_0. \tag{4.78}$$

Due to the definition of C_s we have $-\ln|\sigma_n|^2 \geq 1$ for all $n \in \mathbb{Z}$. Therefore, after possibly redefining c and C, (4.78) holds for all $n \in \mathbb{Z}$, and we obtain

$$C^{-p}(1+n^2)^{-\frac{p+\epsilon}{2}} \leq f_p(|\sigma_n|^2) \leq c^{-p}(1+n^2)^{-\frac{p}{2}}, \qquad n \in \mathbb{Z}. \tag{4.79}$$

The first inequality and (4.71) imply the first inclusion in (4.77) and the mapping properties of $f_p(A^*_{\mathrm{N}} A_{\mathrm{N}}))^{-1}$, and the second inequality accounts for the second inclusion in (4.77) and the mapping properties of $f_p(A^*_{\mathrm{N}} A_{\mathrm{N}})$. ■

Remark 4.21. As for the sound-soft case, the situation is a little simpler for reconstructions from *near field data*. Let $\tilde{A_{\mathrm{N}}}$ be the operator that maps a function $f \in H^s(\partial K_q)$ to $v\big|_{\{|x|=R\}}$ where v is the radiating solution to the Helmholtz equation with Neumann boundary values $\frac{\partial v}{\partial \nu}|_{\partial K_q} = f$. Then, under the assumptions of Theorem 4.20, the operator

$$f_p(\tilde{A_{\mathrm{N}}}^* \tilde{A_{\mathrm{N}}}) : H^s_{\mathbb{C}} \to H^{s+p}_{\mathbb{C}}$$

is bounded and boundedly invertible.

By Theorem 4.20, (4.24) with A_{N} instead of $F'_{\mathrm{N}}[q]$ is a closeness condition with respect to the usual Sobolev norm $\|\cdot\|_{H^{s+p+\epsilon}}$. By arguments similar to those in Subsection 4.4.2. it can be shown that under additional assumptions the singular values of $f_p(F'_{\mathrm{N}}[q]^* F'_{\mathrm{N}})$ have the same asymptotic behavior as the singular values of $f_p(A^*_{\mathrm{N},const} A_{\mathrm{N},const})$ (cf. [Hoh98]).

4.5. Remarks on the nonlinearity condition

Unfortunately, none of the nonlinearity conditions in Section 4.1. could be proved for an inverse scattering problem or the inverse potential problem, yet. Hence no complete convergence proof is available at this time.

An important example to have in mind is the case of concentric circles. For simplicity let us consider the inverse potential problem with $R = 1$ and $s = 0$. If r is the constant function with values $0 < r < 1$, then $F'_{\mathrm{P}}[r] : L^2([0, 2\pi]) \to L^2([0, 2\pi])$ is the self-adjoint operator which multiplies the lth Fourier mode by $r^{|l|}$. Hence, $F'_{\mathrm{P}}[r^\lambda] = F'_{\mathrm{P}}[r]^\lambda$ for $\lambda > 0$. This shows that for $F = F_{\mathrm{P}}$, $x = r$ and $x^\dagger = r^2$ neither the Newton- Mysovskii condition (4.8) nor the conditions $F'[x] = R(x, x^\dagger)F'[x^\dagger]$ or $F'[x] = F'[x^\dagger]R(x, x^\dagger)$ are satisfied for a bounded operator $R(x, x^\dagger)$ (cf. [HNS95], [Kal97]). Note that even though $F'_{\mathrm{P}}[r^2] = F'_{\mathrm{P}}[r]^2$ is infinitely more smoothing than $F'_{\mathrm{P}}[r]$, the corresponding operators in (4.24) only differ by a constant:

$$f_p(F'_{\mathrm{P}}[r^2]) = 2^{-p} f_p(F'_{\mathrm{P}}[r]).$$

Note that for ill-posed problems the estimate (4.6) on the Taylor remainder is a much stronger condition than the simple estimate $C\|x - \bar{x}\|^2$ since $\|F(x) - F(\bar{x})\|$ may be much smaller than $\|x - \bar{x}\|^2$. For a discussion of the relationships between the different nonlinearity conditions we refer to [HS94], [HHS95] and [DES98].

We do not have much hope that either (4.6) or (4.18) can be shown for inverse scattering problems. However, the main idea in the convergence proofs

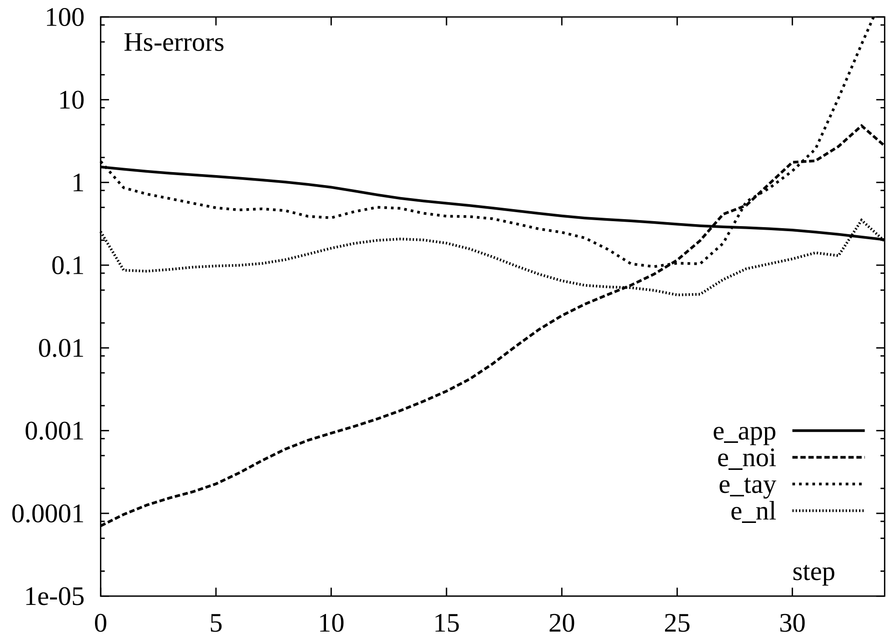


Figure 4.3: Error components for the IRGNM

in Sections 4.2. and 4.3. is the splitting of the total error into several components which can be analyzed separately. Using (4.18) is only one possible way to estimate the nonlinearity terms. One may try to find other estimates of these terms that use specific properties of inverse scattering problems.

Fig. 4.3 shows a plot of the error terms in our analysis. We used the operator F_{N} with $\delta = 0.0001$ and a bean-shaped curve defined on p. 121. With the discrepancy principle with $\tau = 2$ the iteration would have been stopped after $N = 18$ iterations. It is encouraging that the nonlinearity terms e_n^{tay} and e_n^{nl} are clearly smaller than the approximation error e_n^{app} for $n \leq N$.

5. Numerical results

In this final chapter we report on some numerical experiments illustrating the theoretical results of the previous chapters. We compare the performance of different iterative regularization methods for inverse obstacle scattering problems and study the rates of convergence of the IRGNM. Finally, we look at some modifications of the standard situation which are important from a practical point of view and make reconstructions more difficult.

5.1. Implementation and comparison

The implementation of the operators $F_{\mathrm{P}}, F_{\mathrm{D}}$, and F_{N}, their derivatives and the adjoints of these derivatives has been described in Chapter 2 and Section 4.4.. Here we focus on the implementation of iterative regularization methods.

We have designed a general C++-class library for iterative regularization methods that has been used in all our numerical experiments. In our implementation we have used the FFT-Code from [FJ99], and the Bessel functions from `http://www.netlib.org/cephes`.

Implementation of Landweber iteration and Newton methods with inner iteration. It turns out that it is quite important to work with the right function spaces for numerical realizations just as well as for theoretical investigation. Recall that we have established Fréchet differentiability of the scattering problem solution operators F_{D} and F_{N} with respect to the $\|\cdot\|_{C^1}$-norm and differentiability of the potential problem solution F_{P} with respect to the $\|\cdot\|_{\infty}$-norm. Since we need a Hilbert space structure, we have chosen $X = H^s([0, 2\pi])$ with $s > 1.5$ for F_{D} and F_{N} and $s > 0.5$ for F_{P}. For the choice $X = L^2([0, 2\pi])$ the reconstructions of obstacles are typically either unstable or less accurate. For the Levenberg-Marquardt algorithm and similar methods we observed serious stability problems for more than about 15 degrees of freedom with $X = L^2([0, 2\pi])$. Even for Landweber iteration, which is the most stable of the regularization methods considered here, the iterates are perturbed by oscillations in many cases (cf. Fig. 5.1). For both Landweber iteration and the Newton-CG method the reconstructions are almost always significantly better for $X = H^s([0, 2\pi])$, $s > 1.5$ than for $X = L^2([0, 2\pi])$.

In all the experiments reported here we chose $s = 1.6$ for F_{D} and F_{N} and $s = 0.6$ for F_{P}. The choices $s = 1, 2, 3$ also work well in many cases. However, our choice of s seems to be a good compromise between stability and smallness of the initial error.

To implement Landweber iteration and Newton methods with inner iterations in $H^s([0, 2\pi])$ we represent periodic functions on $[0, 2\pi]$ by their weighted Fourier coefficients. Consider real or complex trigonometric polynomials of the form

$$p(t) = \frac{a_0}{\sqrt{2\pi}} + \frac{1}{\sqrt{\pi}} \sum_{j=1}^{n-1} (a_j \cos jt + b_j \sin jt) + \frac{a_n}{\sqrt{2\pi}} (\cos nt + \sin nt). \quad (5.1)$$

We will comment on this choice of spaces, which is slightly different from (2.16), in a moment. The coefficients a_j and b_j can be computed from the vector $\underline{p} = \sqrt{\frac{\pi}{n}} \left(p(t_k^{(n)}) \right)_{0..2n-1}$ of values at the grid points $t_k^{(n)} := \frac{k\pi}{n}$ with time complexity $\mathrm{O}(n \ln n)$ as follows: The Fast Fourier Transform (FFT) yields a vector $\underline{c} = (c_j)_{0..2n-1}$ such that

$$p_j = \frac{1}{\sqrt{2n}} \sum_{j=0}^{2n-1} c_j \exp(\mathrm{i} j t_k^{(n)}).$$

As $\exp(\mathrm{i} j t_k^{(n)}) = \exp(\mathrm{i}(j - 2n) t_k^{(n)})$ and $\sin(n t_k^{(n)}) = 0$ for all $j, k \in \mathbb{N}_0$, the coefficients a_j and b_j are given by

$$\begin{aligned} a_0 &= c_0, \quad a_n = c_n, \\ a_j &= \frac{1}{\sqrt{2}} (c_j + c_{2n-j}), \quad b_j = \frac{\mathrm{i}}{\sqrt{2}} (c_j - c_{2n-j}), \quad j = 1, \dots n-1. \end{aligned}$$

Since FFT is a unitary mapping, it follows that

$$|\underline{p}|^2 = |\underline{c}|^2 = \sum_{j=0}^{n} |a_j|^2 + \sum_{j=1}^{n-1} |b_j|^2 = \|p\|_{L^2}^2. \quad (5.2)$$

Moreover, the real $2n \times 2n$-matrix O defined by

$$O\underline{p} = (a_0, a_1, b_1, \dots, a_{n-1}, b_{n-1}, a_n)$$

is orthogonal.

The property (5.2) distinguishes general trigonometric polynomials of the form (5.1) from trigonometric polynomials of the form (2.16). (Of course, the polynomials (2.16) have the property (5.2) with respect to a shifted set of grid points.) Since $\sin nt_k^{(n)} = 0$, it can be seen that the choice (5.1) leads to the same finite dimensional systems (2.21) and (2.22) as (2.16). Whereas the property (5.2) is desirable in the present context of representing norms and scalar products, the simpler form (2.16) was more convenient in Chapter 2.

Introducing the diagonal matrix

$$\begin{aligned} D_s &= \operatorname{diag}\left(((1+[(j+1)/2]^2)^{s/2})_{0..2n-1}\right) \\ &= \operatorname{diag}(1, 2^{s/2}, 2^{s/2}, \ldots, (1+(n-1)^2)^{s/2}, (1+n^2)^{s/2}) \end{aligned}$$

(with $[x] := \sup\{n \in \mathbb{Z} : n \leq x\}$ for $x \in \mathbb{R}$) and $B_s := D_s O$, we can write the Sobolev norm of p as

$$\|p\|_{H^s} = |B_s \underline{p}|.$$

Let $F'[q]_{L^2}\underline{h}$ be a discrete approximation to the Fréchet derivative $F'[q]h$ for one of the operators F_{P}, F_{D} or F_{N} with $\underline{h} = \sqrt{\frac{\pi}{n}}(h(t_k^{(n)}))$. To get an implementation in the Sobolev space $H^s([0,2\pi])$, we represent h by the vector $B_s\underline{h}$. Then the Fréchet derivative is given by $F'[q]_{L^2}B_s^{-1}$ and its adjoint by $B_s^{-t}F'[q]_{L^2}^*$. E.g., if q_j is the trigonometric interpolation polynomial with nodal values $\sqrt{\frac{n}{\pi}}\underline{q}_j$, then the discrete form of Landweber iteration is given by

$$\underline{q}_{j+1} := \underline{q}_j + \mu B_s^{-1} B_s^{-t} F'[q_j]_{L^2}^* (y^\delta - F(q_j)), \qquad j = 0, 1, 2, \ldots.$$

This algorithm can be seen as a special case of *regularization with differential operators* which is described for linear problems in [EHN96]. Yet another way to look at it is to regard $B_s^{-1}B_s^{-t} = O^* D_s^{-2} O$ as an implementation of the adjoint $j^* : L^2([0,2\pi]) \to H^s([0,2\pi])$ of the inclusion mapping $j : H^s([0,2\pi]) \hookrightarrow L^2([0,2\pi])$.

The implementation of the application of the matrix O and its adjoint can also be used for trigonometric differentiation which is needed to evaluate the Fréchet derivative of the operator F_{N}.

The performance of Landweber iteration depends critically on the choice of the scaling parameter μ. To facilitate the choice of this parameter, we used the *scaled Landweber iteration*

$$q_{n+1}^\delta := q_n^\delta + \frac{\tilde{\mu}}{\|F'[q_0]\|^2} F'[q_n^\delta]^* (u_\infty^\delta - F(q_n^\delta)).$$

In this form the iteration is *scaling invariant*, i.e. the iterates remain unchanged if the operator F and the data u_∞^δ are replaced by λF and some λu_∞^δ for $\lambda \in \mathbb{C}\backslash\{0\}$ (cf. [DES98]). The parameter $\tilde{\mu}$ has to be chosen such that $\tilde{\mu}\|F'[q]\| \le \|F'[q_0]\|$ for all q in a ball around $q^\dagger$ containing q_0. In all our experiments we used $\tilde{\mu} = 0.8$, and the results did not improve significantly for other values of $\tilde{\mu}$. We approximated $\|F'[q_0]\|^2 = \|F'[q_0]^*F'[q_0]\|$ by a few iterations of the power method $z_{n+1} := \frac{1}{\|z_n\|}F'[q_0]^*F'[q_0]z_n$ with a random start vector z_0. Typically, after a few steps we had $\|z_n\| \approx \|F'[q_0]\|^2$. An alternative way to estimate $\|F'[q_0]\|^2$ is to use the Lanczos methods (cf., e.g., [Pai72]).

For the Newton-CG method we chose $\rho = 0.8$ and a maximum number of $k_{\max} = 200$ inner iterations. The latter restriction was rarely active. We would like to mention that it is essential for the performance of the Newton-CG method that the adjoints $F'[q_n^\delta]^*$ are computed with respect to the same scalar products that are used to compute the coefficients α_k and β_k in the algorithm . Moreover, we recommend to use A_n^* as discrete approximation to $F'[q_n^\delta]^*$, if possible (cf. p. 106).

Implementation of the Levenberg-Marquardt algorithm and the generalized IRGNM. To implement the Levenberg-Marquardt algorithm and the generalized IRGNM we used the variational formulations (4.11) and (4.21). This leads to linear least-squares problems for block systems of the form

$$\begin{pmatrix} A \\ B \end{pmatrix} \bar{h} = \begin{pmatrix} v \\ w \end{pmatrix}. \tag{5.3}$$

Here A and v correspond to the term $\|F'[q_n^\delta]h + F(q_n^\delta) - u_\infty^\delta\|^2$, B and w correspond to the terms $\alpha_n\|h + q_n^\delta - q_0\|^2$ or $\alpha_n\|h\|^2$, rsp., and $\underline{h}$ is the coefficient vector of the update $h(t) = \sum_{j=0}^{N_X-1} \underline{h}_j\eta_j(t)$. $\eta_j \in X$ are some basis functions, and B is some (not necessarily $N_X \times N_X$) matrix such that B^tB is the Gram matrix $(\langle\eta_j, \eta_k\rangle_X)$. Note that $|B\underline{h}|^2 = \|h\|_X^2$.

For the scattering problems we approximated the norm in $Y = L^2(S^1)$ by the trapezoidal rule

$$\|f\|_{L^2}^2 \approx \frac{\pi}{N_Y}\sum_{l=0}^{2N_Y-1}|f(\hat{x}_l)|^2, \qquad \hat{x}_l := \begin{pmatrix} \cos\frac{\pi l}{N_Y} \\ \sin\frac{\pi l}{N_Y} \end{pmatrix}.$$

This leads to the matrix entries

$$A_{2l,j} = \sqrt{\frac{\pi}{N_Y}}\,\mathrm{Re}(F'[q_n^\delta]\eta_j)(\hat{x}_l), \qquad v_{2l} = \sqrt{\frac{\pi}{N_Y}}\,\mathrm{Re}(u_\infty^\delta - F(q_n^\delta))(\hat{x}_l),$$
$$A_{2l+1,j} = \sqrt{\frac{\pi}{N_Y}}\,\mathrm{Im}(F'[q_n^\delta]\eta_j)(\hat{x}_l), \quad v_{2l+1} = \sqrt{\frac{\pi}{N_Y}}\,\mathrm{Im}(u_\infty^\delta - F(q_n^\delta))(\hat{x}_l)$$

($0 \leq l <= 2N_Y - 1$, $0 \leq j \leq N_X - 1$). For the potential problem we used the formula $\|f\|_{L^2}^2 = 2\pi a_0 + \pi \sum_{l=1}^{N_Y}(a_l^2 + b_l^2)$ for $f(t) = a_0 + \sum_{l=1}^{N_Y}(a_l \cos lt + b_k \sin lt)$.

In all the experiments reported here we have chosen trigonometric monomials as basis functions $\eta_j : \eta_0(t) := 1$, $\eta_{2k-1}(t) := \cos kt$, and $\eta_{2k}(t) := \sin kt$ for $k \in \mathbb{N}$. Then B is a diagonal matrix with diagonal entries

$$B_{0,0} = \sqrt{2\pi\alpha_n} \qquad B_{2k-1,2k-1} = B_{2k,2k} = \sqrt{\frac{2\pi\alpha_n}{2}}(1+k^2)^{s/2}.$$

For the IRGNM w_l is the weighted lth Fourier coefficient of $q_0 - q_n$, and for the Levenberg-Marquardt algorithm $w = 0$. We have also experimented with more *localized basis functions* (cf. [Hoh96]) which work better for small N_X if properly chosen. However, if N_X is sufficiently large (about $N_X \geq 30$), the results are almost the same.

The discretization errors of this implementation are discussed in Section 5.3.

Choice of the regularization parameters. The regularization parameter α_n in each step of the Levenberg-Marquardt algorithm and the IRGNM can either be chosen by an a-priori rule like (4.16) or by an a-posteriori rule such as (4.12). Numerical experiments show that both methods yield similar results (cf. Fig. 5.3).

The rule (4.12) has the advantage that only one parameter ρ has to be chosen whereas in (4.16) there are two free parameters α_0 and γ. Moreover, a good choice of α_0 is quite different for different problems, whereas, e.g., $\rho = 0.8$ and $\gamma = 1.5^l$ work well for a wide range of problems. Therefore, we suggest to determine α_0 by (4.12) when using (4.16). This was done in all the experiments reported here.

For test purposes we used a simple bisection algorithm to find an approximate solution α_n to (4.12). A more efficient implementation using a Newton method in $1/\alpha_n$ and a bidiagonalization procedure is described in [EHN96, Chap. 9].

Inverse crimes. Since for many direct problems neither explicit solutions nor measurement data are available, synthetic data have to be produced to test numerical algorithms for the inverse problems. If these synthetic data are obtained by the same method that is used in the algorithm for the inverse problem, one often obtains unrealistically good results, especially if the exact solution is chosen from the approximating subspace. The reason is that the errors produced by the direct solver match exactly the errors in the synthetic data, and therefore the problem is reduced to the simple inversion of a finite dimensional system. Such a procedure is often called an *inverse crime*.

To make our tests reliable, we took the following precautions against inverse crimes. We made sure that our exact solution was never in the finite-dimensional approximating subspace. For inverse scattering problems we used a different ansatz and a different number of grid points on the boundary to produce synthetic data. Similarly, we used a much higher number of grid points to compute synthetic data for the potential problem.

Choice of parameters. If nothing else is said we always used $2N_Y = 64$ collocation points for the far field pattern, $2N_g = 128$ grid points, and the wave number $\kappa = 1$ in our experiments with inverse scattering problems.

For the potential problem we used $2N_Y + 1 = 129$ Fourier coefficients, $2N_g = 128$ grid points, and a radius $R = 2$.

To recover the radial function $q^\dagger$ we started from the unit circle $q_0(t) = 1$ and used $N_X = 64$ trigonometric basis functions. As mentioned above, the distance between curves was measured in the Sobolev norm $\|\cdot\|_{H^s}$ with $s = 1.6$ for scattering problems and $s = 0.6$ for the potential problem.

As test examples we chose the bean-shaped curve q_b, the peanut-shaped curve q_p, the rounded rectangle q_r, the star-shaped curve q_s, and the kite-shaped curve z_k which are defined by

$$\begin{aligned}
q_\mathrm{b}(t) &:= \frac{1 + 0.9\cos t + 0.1\sin t}{1 + 0.75\cos t}, \\
q_\mathrm{p}(t) &:= \sqrt{\cos^2 t + 0.26\sin^2(t + 0.5)}, \\
q_\mathrm{r}(t) &:= \left((\cos t)^{10} + \left(\frac{2}{3}\sin t\right)^{10} \right)^{-0.1}, \\
q_\mathrm{s}(t) &:= 0.6 + 0.2\mathrm{e}^{1.4\cos(3t-2) + 0.4\sin t}, \\
z_\mathrm{k}(t) &:= \begin{pmatrix} \cos t + 0.26\cos 2t - 0.65 \\ 1.5\sin t \end{pmatrix}.
\end{aligned}$$

Comparison for exact data. From the convergence plots in Fig. 5.5 and from the pictures in Fig. 5.6 it is clear that Landweber iteration is by far the slowest method. It turns out that (4.7) describes the convergence behavior correctly even though the Newton- Mysovskii condition under which it was derived is not satisfied. This can be seen in Fig. 5.2: the plot of $\ln \|x_n^\delta - x^\dagger\|$ over $\ln(-\ln n)$ is almost linear. It follows from (4.7), (4.16) and (4.33) that the number of Landweber steps that is necessary to achieve the accuracy of n IRGNM steps increases *exponentially* with n! Nevertheless, one can obtain quite accurate reconstructions with Landweber iteration after very many iterations (cf. Fig. 5.7). Let us mention again that this is not true for $s = 0$, i.e. $X = L^2([0, 2\pi])$. In this case the reconstructions are usually contaminated by oscillations after a certain number of iterations even for exact data (cf. Fig. 5.1).

The Newton-CG method makes remarkably good progress in the beginning in reducing low frequency components of the error. It is much faster than Landweber iteration, but the asymptotic speed of convergence is clearly slower than that of the Levenberg-Marquardt algorithm and the IRGNM.

The Levenberg-Marquardt algorithm and the IRGNM are quite similar if the regularization parameters α_n are chosen the same way. Usually, the Levenberg-Marquardt algorithm gives better results at the beginning whereas the IRGNM is better in the long run (cf. Fig. 5.5). Moreover, as discussed after (4.17), the IRGNM is more stable than the Levenberg-Marquardt algorithm. This is exhibited in Fig. 5.4 where we used only $2N_g = 64$ grid points instead of our default value $2N_g = 128$. The reconstructions of the Levenberg-Marquardt algorithm explode before those of the IRGNM, and the error at the time before divergence takes place is larger. Because of this increased stability and because of the more complete convergence analysis, we prefer the IRGNM over the Levenberg-Marquardt algorithm.

The generalized IRGNM introduced in Section 4.1. is clearly the fastest of all the methods discussed here. After 60 iterations in the first plot of Fig. 5.5 and after 33 iterations in the second plot the residual was about as small as the computational errors and the iteration diverged.

For the sound-hard scattering problem with our standard choice of parameters 50 iteration steps took 14.4 seconds for Landweber iteration, 22.3 seconds for the Newton-CG method, 28.9 seconds for the IRGNM, and 29.1 seconds for the generalized IRGNM with $l = 3$ inner iteration on an SGI R10000 machine. For the potential problem the corresponding computation times were 1.15, 10.0, 9.3 and 9.4 seconds. The difference between Landweber iteration and Newton methods is much more pronounced for the potential problem since no matrix has to be inverted to evaluate the solution operator.

Comparison for noisy data. Let us now look at the performance of iterative regularization methods in the presence of data noise errors. Here we have always worked with pseudo-random noise (cf. §5.4.2.). Moreover, we have used the discrepancy principle (4.4) with $\tau = 1.2$ to stop the iteration. Although this choice of τ is not yet supported by theory for nonlinear problems, the iteration was terminated before divergence in all our experiments, and the results were better than with larger values of τ.

Fig. 5.7 and 5.8 show that all things considered the results of different methods are of similar quality for noisy data. This holds true in particular for Landweber iteration and the generalized IRGNM. The Newton-CG method yields more accurate results in some cases (as in Fig. 5.7c), 10% noise) at the cost of stability (cf. Fig. 5.7b), 1% noise and Fig. 5.8). In Fig. 5.8 the results obtained with the generalized IRGNM ($l = 3$) are slightly better than the results obtained with the standard IRGNM ($l = 1$).

Although the results of different methods are similar, the computation times to achieve these results are quite different. Whereas Landweber iteration needs 10000 and more iterations until the stopping criterion (4.4) is satisfied for 1% noise, Newton methods need no more than 30 iterations. For noise levels of 1 to 10% usually the Newton-CG method was fastest in our test examples, followed by the generalized IRGNM.

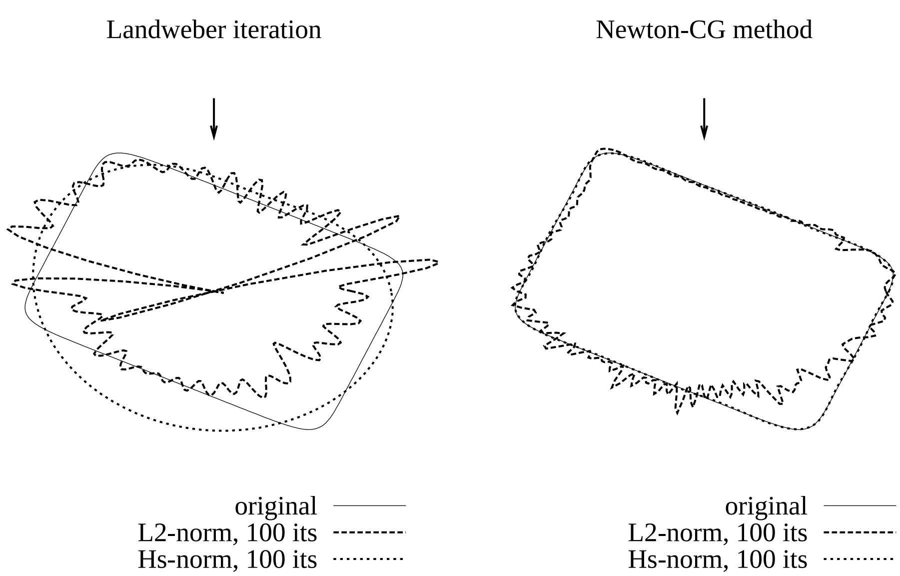


Figure 5.1: Stability of regularization methods with L^2-norm versus H^s-norm in X; $F = F_{\mathrm{D}}$; $q^\dagger(t) = q_{\mathrm{r}}(t+2)$; $\delta = 0$

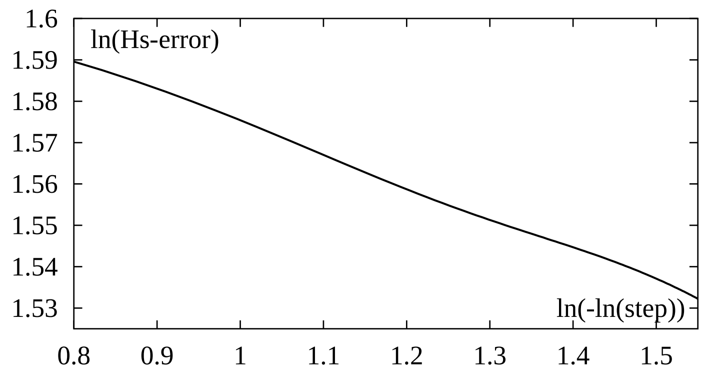


Figure 5.2: Speed of convergence of Landweber iteration; $F = F_{\mathrm{D}}$; $d = (1,0)$; $q^{\dagger} = q_{\mathrm{r}}$, $\delta = 0$

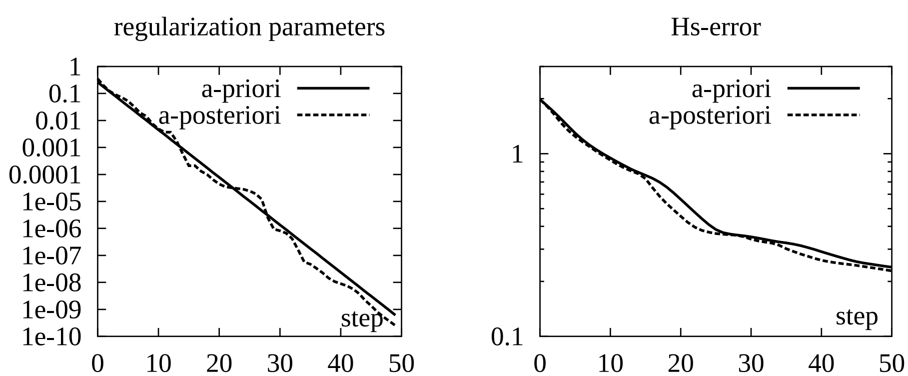


Figure 5.3: Levenberg-Marquardt algorithm with a-priori and a-posteriori choice of α_n; $F = F_{\mathrm{N}}$; $d = (1,0)$; $q = q_{\mathrm{b}}$; $\delta = 0$; $\rho = 0.75$

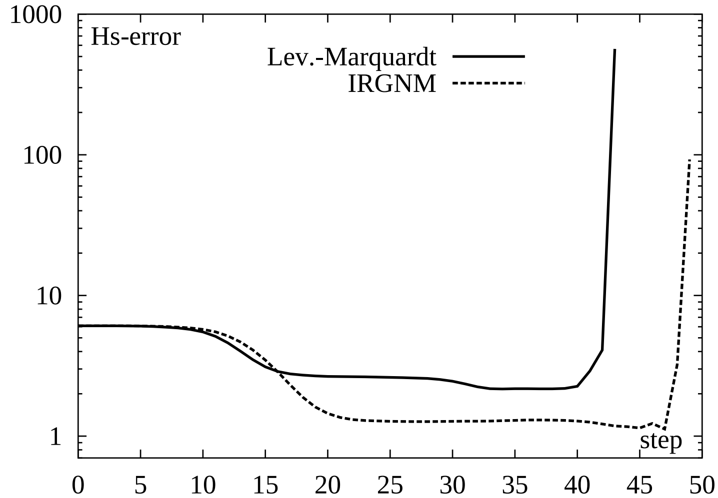
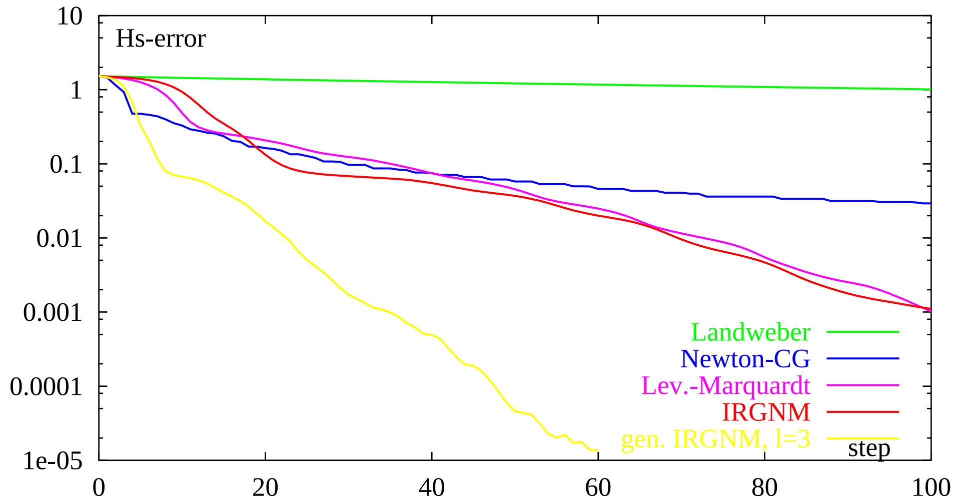
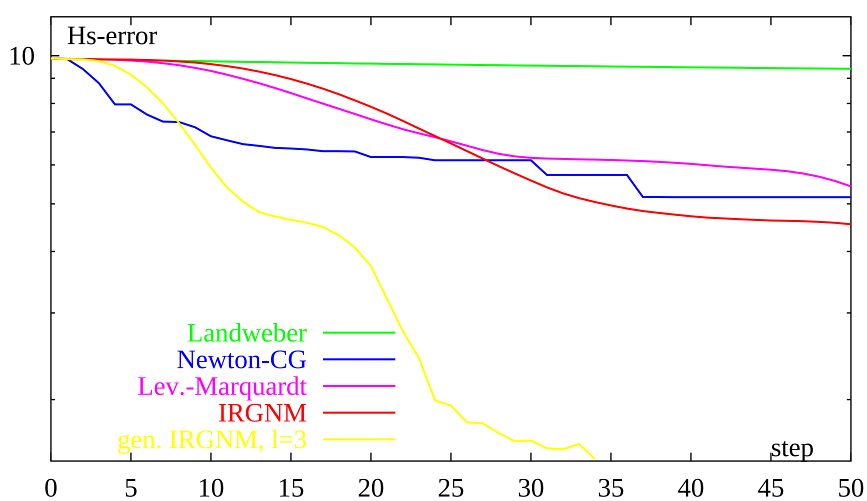


Figure 5.4: Comparison of stability of Levenberg-Marquardt algorithm and IRGNM; $F = F_{\mathrm{D}}$; $q^{\dagger} = q_{\mathrm{s}}$, $\delta = 0$; $N_g = 32$ instead of default $N_g = 64$



$F = F_{\mathrm{P}};\ q^{\dagger} = q_{\mathrm{s}}$



$F = F_{\mathrm{D}};\ z_{q^{\dagger}} = z_{\mathrm{k}};\ d = (1, 0)$

Figure 5.5: Comparison of convergence plots for different methods with exact data

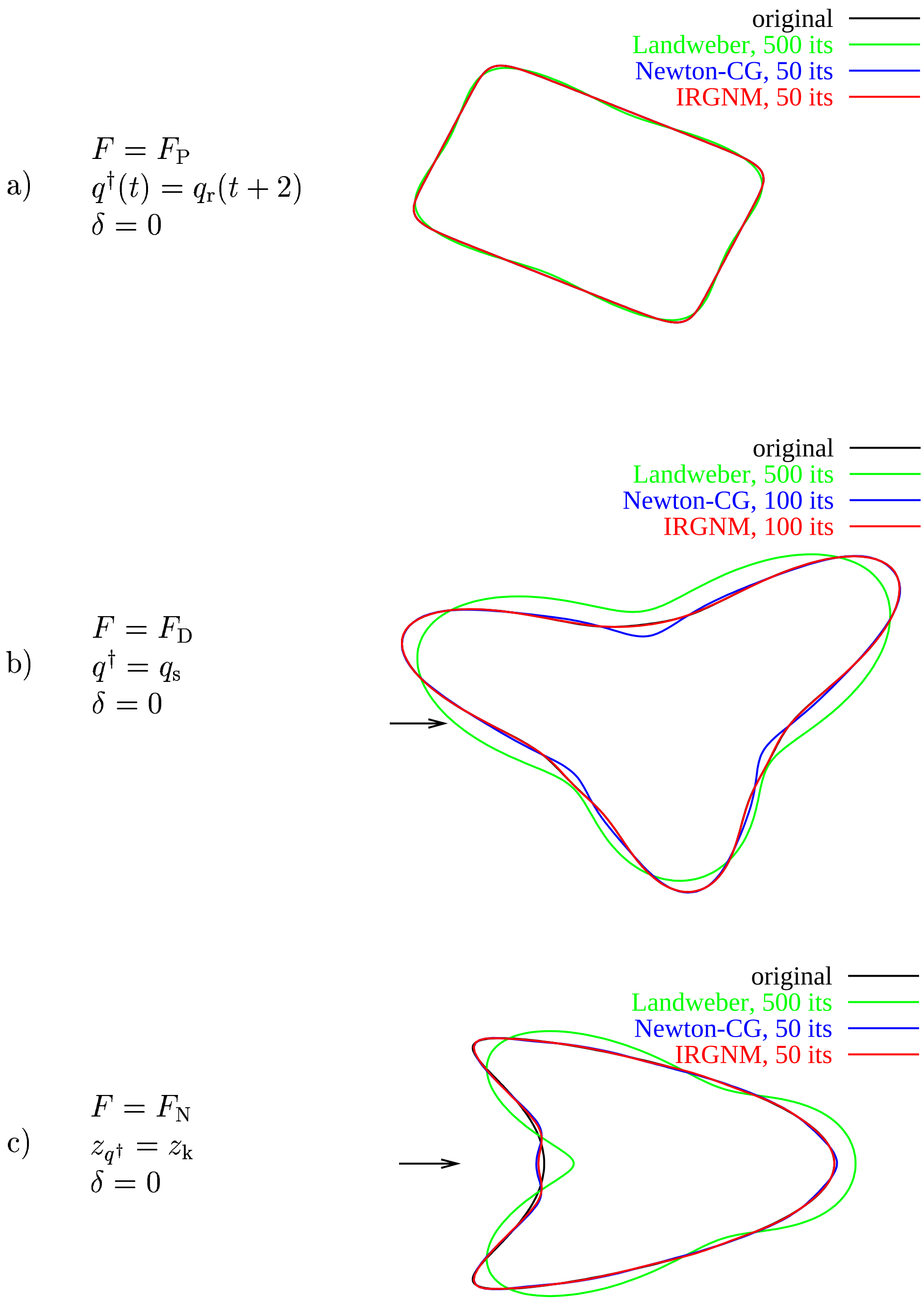
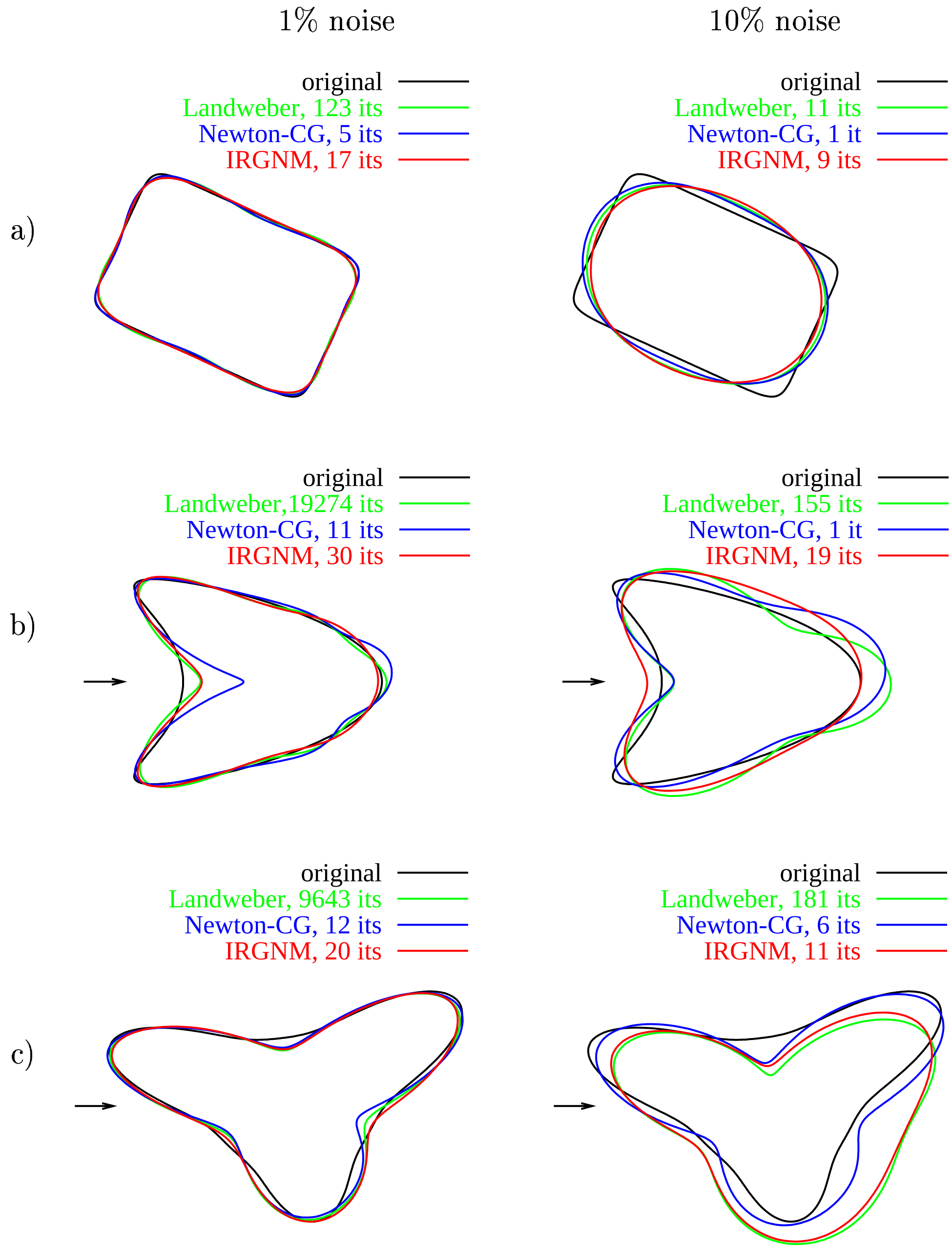


Figure 5.6: Comparison of methods for exact data



a) $F = F_{\mathrm{P}}$, $q^{\dagger}(t) = q_{\mathrm{r}}(t+2)$
b) $F = F_{\mathrm{D}}$, $z_q^{\dagger} = z_{\mathrm{k}}$
c) $F = F_{\mathrm{N}}$, $q^{\dagger} = q_{\mathrm{s}}$

Figure 5.7: Comparison of methods for noisy data

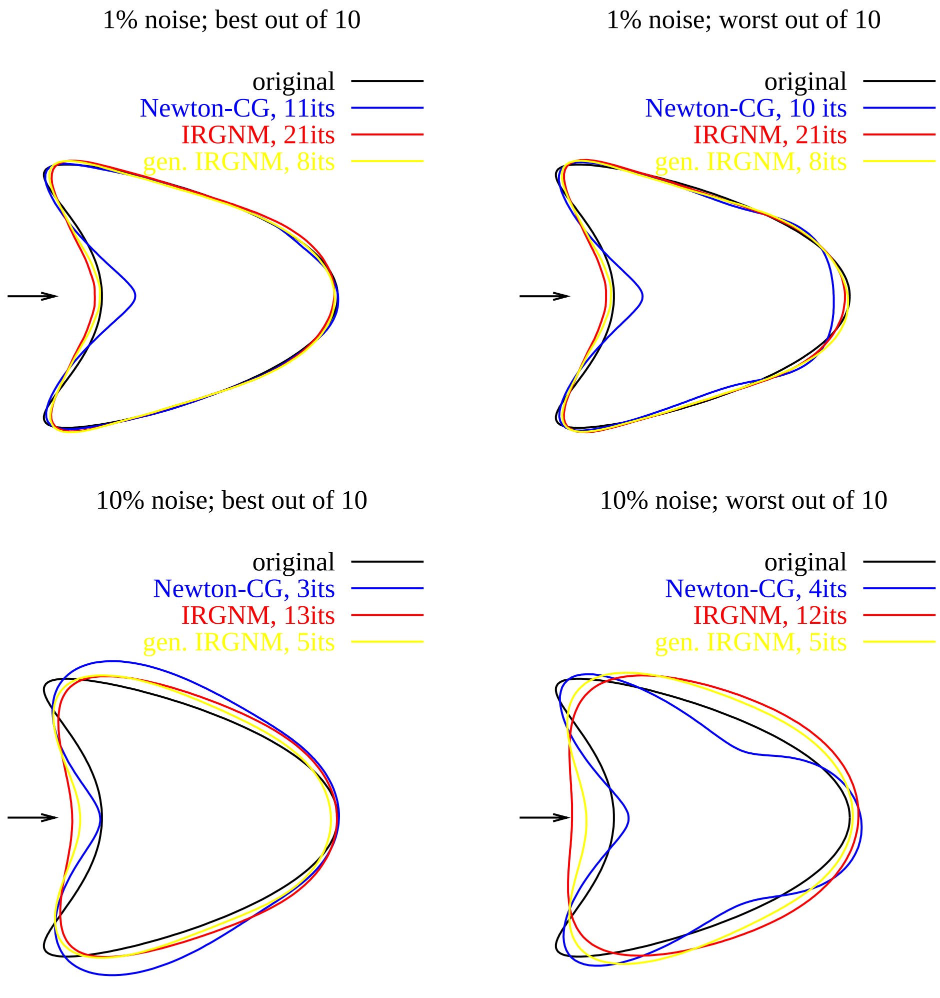


Figure 5.8: Comparison of Newton-CG method, IRGNM and generalized IRGNM with $l = 3$ for noisy data; $F = F_{\mathrm{D}}$; $z_{q^\dagger} = z_{\mathrm{k}}$

5.2. Convergence rates for the IRGNM

In this section we describe numerical experiments that verify the theoretical results from Sections 4.2. and 4.3.. (4.16) and (4.33) imply the estimate

$$\begin{aligned}\ln\|q_n - q^\dagger\|_{H^s} &\leq \ln(C(-\ln\frac{\gamma^{-n}}{\mathrm{e}})^{-p}) \leq \ln(C'(n\ln\gamma)^{-p}) \\ &= (\ln C' - p\ln\ln\gamma) - p\ln n\end{aligned}$$

for exact data. Hence we expect a plot of $\ln\|q_n - q^\dagger\|_{H^s}$ over $\ln n$ to be asymptotically close to a straight line. Similarly, for noisy data we have

$$\ln\|q_{N(\delta,g^\delta)} - q^\dagger\| \leq \ln(C(-\ln\delta)^{-p}) = \ln C - p\ln(-\ln\delta).$$

due to (4.38) and (4.40), and therefore, we expect a plot of $\ln\|q_N(\delta, u_\infty^\delta) - q^\dagger\|_{H^s}$ over $\ln(-\ln\delta)$ to be asymptotically linear. These predictions are confirmed in Fig. 5.9, 5.10, and 5.11.

Moreover, according to our theoretical results the parameter p in the source condition (4.24) corresponds to the negative slopes of the asymptotic straight lines in Fig. 5.9, 5.10, and 5.11, and that p is related to the smoothness of $q^\dagger - q_0$. In order to test these predictions, we constructed curves $q^\dagger$ with exactly known smoothness as follows: Let $f * g$ denote the convolution of 2π-periodic functions f, g, i.e. $(f * g)(t) := \int_{-\pi}^{\pi} f(s)g(t-s)\,\mathrm{d}s$, and let $f^{[m]} := f * \cdots * f$ be the m-fold convolution of f. We define f_a as the 2π-periodic extension of the characteristic function of the interval $[-a, a]$. It can be shown by induction that $f_a^{[m]} \in C^{m-2}([0, 2\pi])$ for $m \geq 2$ and $a < \pi/m$ and that the m-th derivative of $f^{[m]}$ is piecewise constant, i.e. $f_a^{[m]} \notin C^{m-1}([0, 2\pi])$. Hence Sobolev's embedding lemma implies $f_a^{[m]} \notin H^p([0, 2\pi])$ for $p > m - \frac{1}{2}$. On the other hand, calculating the Fourier coefficients of f_a explicitly and using the fact that the Fourier coefficients of $f * g$ are given by products of the Fourier coefficients of f and g, it can be shown that $f^{[m]} \in H^p([0, 2\pi])$ for $p < m - \frac{1}{2}$.

We chose the test curves $q_{[m]} := 1 + cf_a^{[m]}$ with $a = \frac{1}{m}$ and c such that $q_{[m]}(0) = \frac{5}{4}$. These curves describe local perturbations of the unit circle which look almost identical, but have different smoothness (cf. Fig 5.9). As usual we used the unit circle $q_0 \equiv 1$ as initial guess.

From the results in Section 4.4. we expect that $p \approx \sup\{p' : q_{[m]} - q_0 \in H^{s+p'}\} = m - 0.5 - s$. In Tab. 5.1 we listed the slopes of the linear regression lines for plots corresponding of $\ln\|q_n - q^\dagger\|$ over $\ln n$ ($n = 20, \ldots 60$) and for plots of $\ln\|q_N(\delta, u_\infty^\delta) - q^\dagger\|_{H^s}$ over $\ln(-\ln\delta)$ ($10^{-8} < \delta \leq 5\cdot 10^{-4}$). Whereas in the first case ($\delta = 0$) the slope are quite close the predicted values, in the second case ($\delta > 0$) the slopes are a bit smaller than expected. However, it is clearly exhibited that more smoothness leads to faster convergence, and the results are of the expected order.

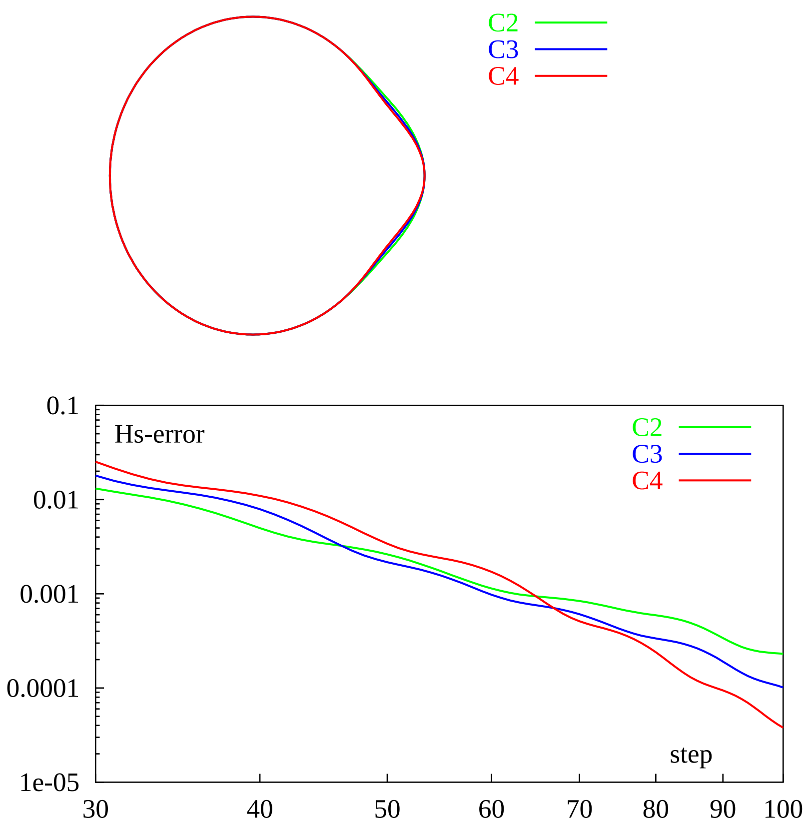


Figure 5.9: Speed of convergence for perturbations of the unit circle; $F = F_{\mathrm{P}}$; $\delta = 0$

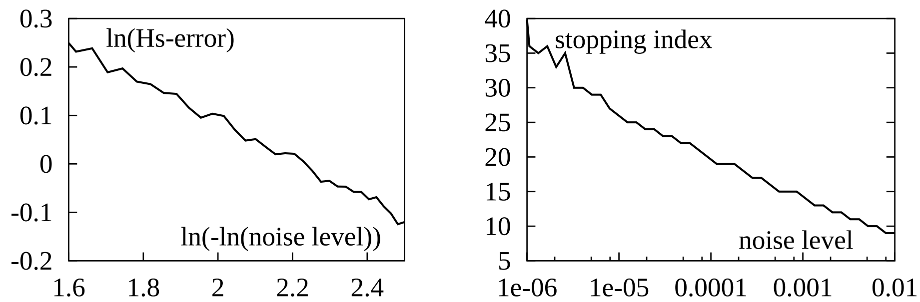


Figure 5.10: Convergence rates for the generalized IRGNM with discrepancy principle; $F = F_{\mathrm{D}}$; $d = (1, 0)$; $q^{\dagger} = q_{\mathrm{b}}$

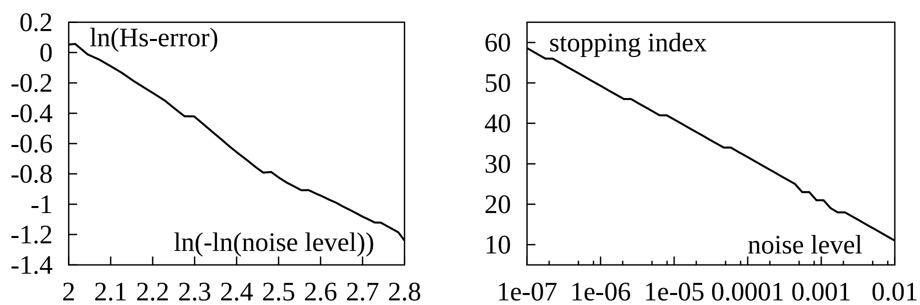


Figure 5.11: Convergence rates for the IRGNM with discrepancy principle; $F = F_{\mathrm{N}}$; $d = (1, 0)$; $q^{\dagger} = q_{\mathrm{b}}$

$F = F_{\mathrm{P}}$
$s = 1$

$q^\dagger$	$\sup\{p : q^\dagger \in H^{1+p}\}$	$\delta = 0$	$\delta > 0$
$q_{[2]}$	0.5	-0.47	-0.83
$q_{[3]}$	1.5	-1.28	-2.22
$q_{[4]}$	2.5	-2.09	-3.75
$q_{[5]}$	3.5	-3.14	-5.78
$q_{[6]}$	4.5	-4.33	-5.97

$F = F_{\mathrm{N}}$
$s = 3$

$q^\dagger$	$\sup\{p : q^\dagger \in H^{3+p}\}$	$\delta = 0$	$\delta > 0$
$q_{[4]}$	0.5	-0.4	-0.9
$q_{[5]}$	1.5	-1.8	-2.7
$q_{[6]}$	2.5	-2.4	-3.3

Table 5.1: slopes of the regression lines for exact data convergence plots ($n = 20 \dots 60$) and for convergence rates plots ($10^{-8} < \delta \leq 5 \cdot 10^{-4}$)

5.3. Adapting the discretization parameters during the iteration

Let us first identify the operators $F^{(n)}$ and $A_q^{(n)}$ in Section 4.2. for our implementations of the scattering problems. (The potential problem is treated analogously.) Let $\tilde{F}_{N_g} : D(F) \to L^2_{\mathbb{C}}(S^1)$ and $\tilde{A}_{q,N_g} : H^s_{\mathbb{R}}([0,2\pi]) \to L^2_{\mathbb{C}}(S^1)$ be the approximations to F and $F'[q]$ with $2N_g$ grid points as described in Chapter 2. Here either $F = F_{\mathrm{D}}$ or $F = F_{\mathrm{N}}$. Let P_{N_X} be the orthogonal projection onto $\mathrm{span}\{\eta_j : j = 0, \dots, 2N_X\}$. Moreover, let $\hat{Q}_{N_Y}$ be the trigonometric interpolation operator on S^1 with respect to the $2N_Y$ equidistant interpolation points $\hat{x}_l^{(N_Y)} := (\cos \frac{l\pi}{N_Y}, \sin \frac{l\pi}{N_Y})$, $l = 0, \dots, 2N_Y - 1$ analogous to the operator P_n in (2.18). Then the operator

$$Q_{N_Y} f := \sqrt{\hat{Q}_{N_Y}((\mathrm{Re}\, f)^2)} + \mathrm{i}\sqrt{\hat{Q}_{N_Y}((\mathrm{Im}\, f)^2)}$$

satisfies

$$\|Q_{N_Y} f\|^2_{L^2} = \frac{\pi}{N_Y} \sum_{l=0}^{2N_Y-1} |Q_{N_Y} f(\hat{x}_l^{(N_Y)})|^2$$

since the trapezoidal rule with $2N_Y$ grid points is exact for trigonometric polynomials of degree $\leq N_Y$. Therefore, we may interpret collocating at the points $\hat{x}_l^{(N_Y)}$ and then taking the discrete l^2-norm as applying the operator Q_{N_Y} and then integrating exactly. Hence, our approximations to F and A_q are

$$\begin{aligned} F^{(n)}(q) &:= Q_{N_Y(n)} \tilde{F}_{N_g(n)}(q) \qquad \text{and} \\ A_q^{(n)} &:= Q_{N_Y(n)} \tilde{A}_{q,N_g(n)} P_{N_X(n)}. \end{aligned}$$

The approximation errors can be estimated by the triangle inequality as follows:

$$\begin{aligned} \|F^{(n)}(q) - F(q)\| &\leq \|(Q_{N_Y} - I)\tilde{F}_{N_g}(q)\| + \|\tilde{F}_{N_g}(q) - F(q)\| \\ \|A_q^{(n)} - F'[q]\| &\leq \|(Q_{N_Y} - I)\tilde{A}_{q,N_g} P_{N_X}\| \\ &\quad + \|\tilde{A}_{q,N_g}(P_{N_X} - I)\| + \|\tilde{A}_{q,N_g} - F'[q]\| \end{aligned}$$

Here we have omitted the argument (n) of the discretization indices N_g, N_X, and N_Y. If $f : S^1 \to \mathbb{R}$ is an analytic function, the trigonometric interpolation error satisfies

$$\|(I - \hat{Q}_{N_X})f\|_\infty = \mathrm{O}\left(\exp(-sN_X)\right)$$

where s corresponds to the width of the strip in the complex plane to which the periodic function $t \mapsto f(\cos t, \sin t)$ can be extended analytically (cf. [Kre89, Theorem 11.5]). Consequently,

$$\|(I - Q_{N_X})f\|_{L^2} = \mathrm{O}\left(\exp(-(sN_X)/2)\right).$$

It can be shown that the periodic functions corresponding to far field patterns can be analytically extended to the entire plane, i.e. the previous estimate holds for any $s > 0$ if f is a far field pattern. The size of the other error terms depends on the smoothness of q. If q is analytic, it can be shown that $\|\tilde{F}_{N_g}(q) - F(q)\|$ and $\|\tilde{A}_{q,N_g} - F'[q]\|$ decay exponentially (cf. [Kre89, Kre95c, Hoh98]). Since P_{N_X} is a trigonometric projection operator, the term $\|\tilde{A}_{q,N_g}(I - P_{N_X})\| = \|(I - P_{N_X})\tilde{A}^*_{q,N_g}\|$ also decays exponentially due to the characterization of $\tilde{A}^*_{q,N_g}$ in Propositions 4.16 and 4.19. Since our computed iterates q_n^δ are trigonometric polynomials and hence analytic, this suggests that the discretization indices $N_g(n), N_X(n)$ and $N_Y(n)$ should be chosen of the form $a + bn$ with constants $a, b > 0$ such that (4.22a) and (4.22c) are satisfied with an error level $h_n = \mathrm{O}\left(\exp(-n)\right)$. A rigorous analysis would have to take into account that although the iterates q_n^δ are analytic, they converge to a function $q^\dagger$ which is not necessarily analytic, so the width of the strip to which functions can be analytically extended may decrease during the iteration. Such an analysis could take place in Banach spaces of holomorphic functions as introduced in [Kre89, Exercise 12.4.].

In a numerical experiment, we compared the numerical performance of the IRGNM with $N_g(n) = N_X(n) = N_Y(n) = 4 + n$ and $N_g(n) = N_X(n) = N_Y(n) = 64$ over the first 60 iterations. The computation time of the adaptive version is only about a third of the version with fixed discretization parameters whereas the results are almost identical (cf. Fig. 5.12 and Tab. 5.2). Speed-ups of similar order were observed by Ramlau for an adaptive version of Landweber iteration ([Ram99]).

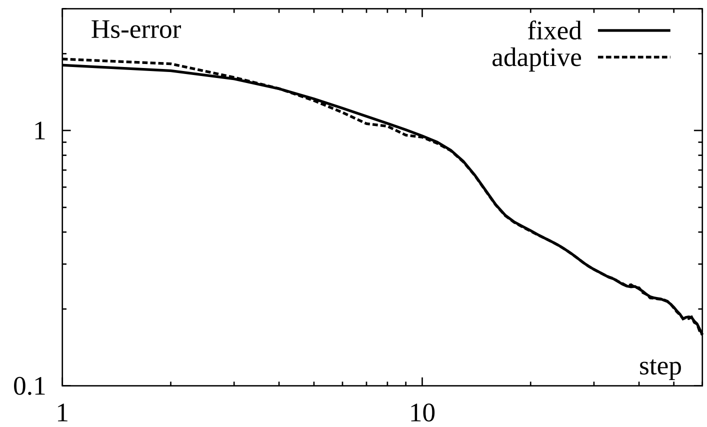


Figure 5.12: Convergence with adaptive choice of discretization parameters; $F = F_{\text{Neum}}$; $d = (1, 0)$; $q^\dagger = q_b$

	fixed	adaptive	
set-up + decomposition of ieq. matrix	47.3%	15.0%	(46.3%)
evaluation of $F^{(n)}(q)$	0.8%	0.2%	(0.5%)
evaluation of $A_n^{(n)}$	41.0%	14.2%	(43.7%)
solution of (5.3)	10.6%	2.5%	(7.5%)
rest	0.4%	0.6%	(2.0%)
total	100.0%	32.5%	(100.0%)

Table 5.2: Computation times with fixed and adaptive choice of discretization parameters

5.4. Miscellaneous

5.4.1. Convergence rates with limited aperture

In many practical situations measurements of the scattered field are not available at all directions, but only at a limited range of angles. Therefore, it is interesting to study how such a lack of information influences the quality of the reconstructions. For test purposes we chose a bean-shaped sound-hard scatterer with one incident plane wave of direction $d = (0, 1)$ and considered far field data in a range of angles centered around the backscattering direction $(0, -1)$. In different experiments the size of this range of angles was 2π (full far field data), π, 0.4π, and 0.2π. In all these experiments we used the same number of data points. Although convergence of the IRGNM is considerably slower for limited-aperture data, one still gets reasonably good reconstructions even for an aperture of only 36 degrees (cf. Fig 5.13).

5.4.2. Random and systematic data errors

In this subsection we look at the influence of the type of the data error on the quality of the reconstructions. In many application the measurement data are contaminated not only by random (e.g. Gaussian distributed) errors, but also by large *systematic errors* due to experimental design or inaccurate mathematical models.

To simulate random measurement errors, we added a computer-generated pseudo-random number to the synthetic data $u_\infty(\hat{x}_j)$ for each $\hat{x}_j$. In Fig. 5.14a) and b) we plotted the best and the worst reconstructions out of 50 experiments with pseudo-random noise. In each case we used the IRGNM stopped according to the discrepancy principle with $\tau = 1.2$. The relative error level was roughly 5%. In Fig. 5.14c) and d) we simulated some simple types of systematic errors. In c) u_∞^δ was given by $(1+\delta)u_\infty$ and d) we had $u_\infty^\delta = (1 + \chi_{\{\hat{x}_2 \geq 0\}} d) u_\infty$ where $\chi_{\{\hat{x}_2 \geq 0\}}$ is the characteristic function of $\{\hat{x} \in S^1 : \hat{x}_2 \geq 0\}$.

These experiments show that reconstructions are usually considerably worse for systematic than for random data errors. This is also true for experiments with various other types of systematic errors that are not reported here, e.g. a large error in a single measurement point or perturbations by trigonometric monomials. Nevertheless, taking into account the severe ill-posedness of the problem, the reconstructions are quite good even for systematic data errors.

5.4.3. Reconstructions with more than one obstacle

In this subsection we consider the reconstruction of scatterers which consist of several components. Each component may have a different boundary condition. In Fig. 5.15 we chose a sound-hard "bean", rotated by 2 and displaced by $(-1.5, 1.5)$, a sound-soft "peanut", rotated by -1 and displaced by $(1.5, -1.5)$, and a sound-hard "rounded rectangle", rotated by 0.5 and displaced by $(0, 2)$. Moreover, we used 8 equidistant incident waves with $\kappa = 1$ and no artificial noise. We used an adaptive choice of the discretization parameters as in Section 5.3.. Again, the reconstruction with the IRGNM is the best, followed by that of the Newton-CG method and that of Landweber iteration.

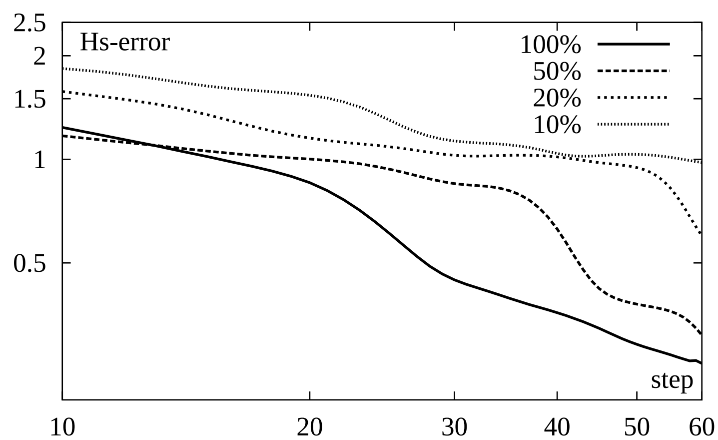


Figure 5.13: Convergence with limited aperture; $F = F_{\mathrm{N}}$; $d = (0, 1)$; $q^{\dagger} = q_{\mathrm{b}}$

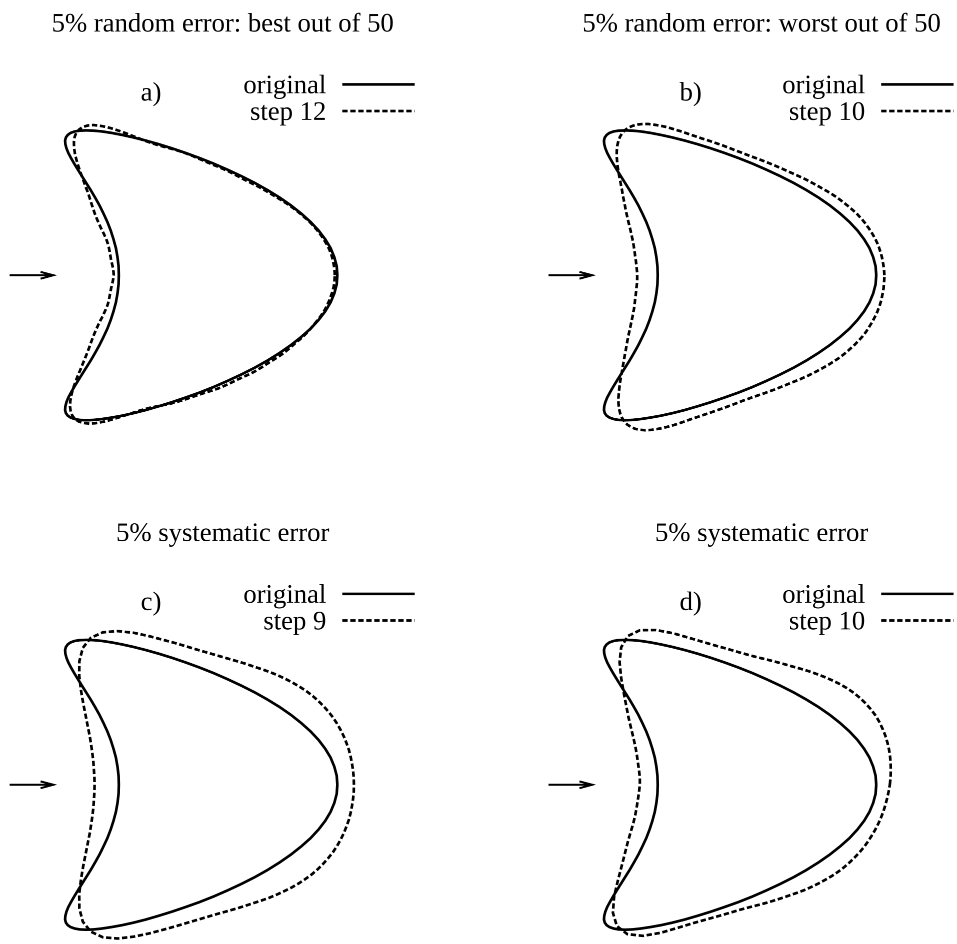


Figure 5.14: Reconstructions with random and systematic data errors; $F = F_{\mathrm{D}}$; $z_{q^\dagger} = z_{\mathrm{k}}$

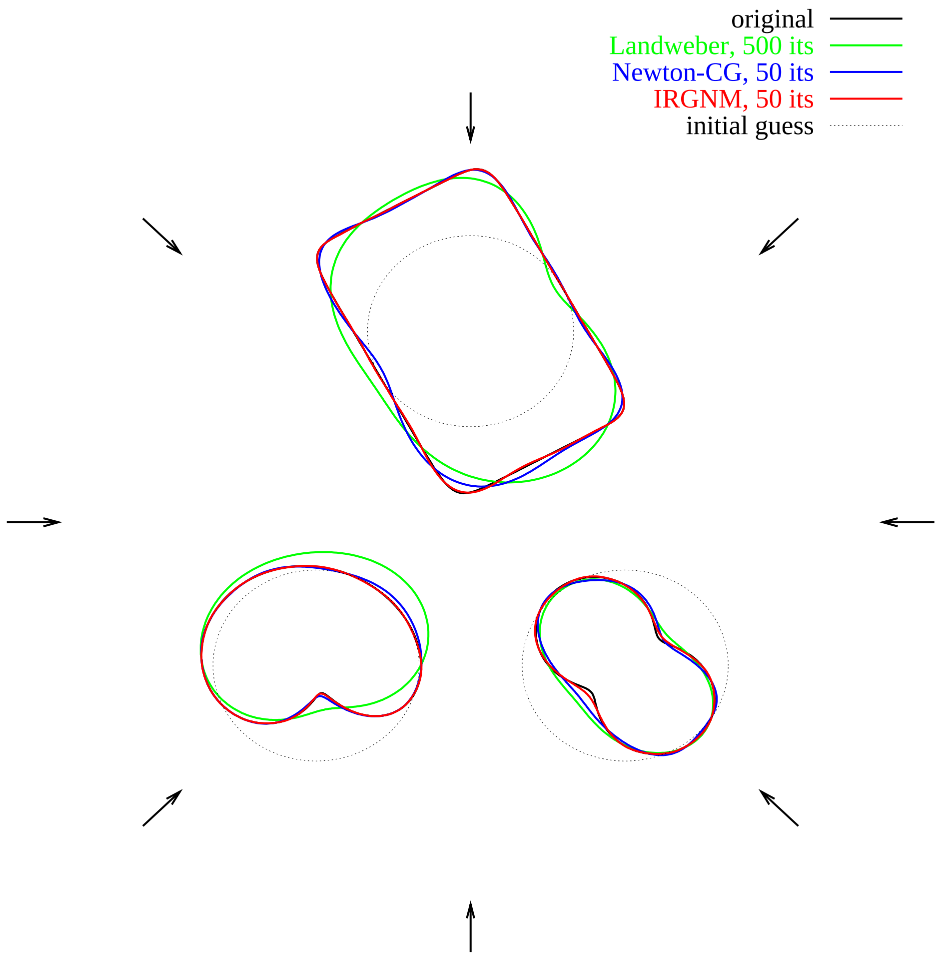


Figure 5.15: Reconstructions with several domains; $\delta = 0$

5.5. Summary

Let us briefly summarize the main results of this chapter. A comparison of iterative regularization methods for inverse scattering problems with exact data shows that the generalized IRGNM introduced in Section 4.1. is the fastest method followed by the standard IRGNM, the Levenberg-Marquardt algorithm, the Newton-CG method and Landweber iteration. The quality of reconstructions with noisy data is similar with all these methods. For noise levels of 1 to 10% the Newton-CG method is usually the fastest, but other methods are more stable.

The estimates on the speed of convergence of the generalized IRGNM derived in Chapter 4 are confirmed in numerical experiments. The results clearly show that the speed of convergence depends on the smoothness of the difference between the exact solution and the initial guess and that the experimental convergence rates are close to the predicted rates.

Although the quality of the reconstructions is impaired considerably if measurement data are available only for a limited range of angles or if they are perturbed by systematic errors, Newton-type methods still yield stable and reasonably good results in these situations. Computation times can be reduced to about a third if the direct solution operator and its derivative are approximated only coarsely as long as the iterates are still far away from the solution. Finally, we have also obtained good reconstructions with more than one scattering obstacle provided the number of obstacles and a sufficiently good initial guess are known. Such an initial guess could be provided by sampling methods as described in [CK96, Pot96a, CPP97, Kir98].

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