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An optimization method for grating profile reconstruction

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Abstract

We consider the inverse diffraction problem to recover a two-dimensional periodic structure from scattered waves measured above the structure. Following an approach by Kirsch and Kress, the inverse problem is reformulated as a nonlinear optimization problem. The resulting Tikhonov regularized least squares problem is then solved iteratively by the Levenberg-Marquardt algorithm. Numerical results for synthetic data demonstrate the practicability of the inversion algorithm. We also present some convergence results for the Tikhonov regularization of the reconstruction problem and for the optimization method.

1 Introduction

The scattering theory in periodic structures has many applications in micro-optics, where periodic structures are often called diffraction gratings. For an introduction to the direct problem of calculating the electromagnetic scattering produced by periodic interfaces, we refer to the monograph [16]. The inverse problem of recovering the periodic structure or the shape of the grating profile from the scattered field is also of great practical importance in modern diffractive optics, e,g,, in quality control and design of diffractive elements with prescribed far field patterns (see [2], [17]).

In this paper, we shall restrict our attention to the simplest case of two-dimensional perfectly conducting gratings and consider the profile reconstruction problem for Dirichlet boundary conditions. Uniqueness results and local stability estimates were obtained in [13], [1], [3], [10], and a result on conditional (global) stability was proved in [4]. Recently, Ito and Reitich [11] proposed a conjugate gradient algorithm based on analytic continuation for the numerical solution of this problem, which appears to be rather efficient for smooth profiles given by a finite Fourier series.

The goal of this paper is to present an alternative algorithm for the inverse Dirichlet problem, following an approach first developed by Kirsch and Kress [14] (see also [7], Chap.5) for acoustic obstacle scattering. In this method, the inverse problem is decomposed into the severely ill-posed linear problem of reconstructing the scattered wave from a knowledge of its far field pattern, and into the well-posed nonlinear problem of determining the unknown profile curve as the location of the zeros of the total field. The discretization of the resulting optimization problem then leads to a nonlinear least squares problem which is solved iteratively by the Levenberg-Marquardt algorithm.

Numerical results are reported for two examples of smooth profiles, where the data are generated using the direct solver of Bruno and Reitich [5]. The computed profiles demonstrate that the numerical performance of our method, whose implementation turns out to be rather easy, is comparable to that of the method used in [11].

We also present a theoretical convergence result for our optimization method, which even holds for general Lipschitz profile curves (see [9] for a detailed presentation). Moreover, for a suitable class of smooth profiles and small wave numbers, we derive a logarithmic convergence rate for the Tikhonov regularized reconstruction problem from the a priori parameter choice of Cheng and Yamamoto [6] and the stability result of [4]. This can be considered as a first step to an error analysis of the reconstruction algorithm.

This paper is organized as follows:

- Section 2. Direct and inverse diffraction problems
- Section 3. Tikhonov regularization
- Section 4. An optimization method
- Section 5. Reconstruction algorithm
- Section 6. Numerical results.

2 Direct and inverse diffraction problems

The scattering of time-harmonic electromagnetic waves in the TE (transverse electric) mode by two-dimensional perfectly reflecting periodic structures is modelled by the Dirichlet problem for the Helmholtz equation. Let the profile of the diffraction grating be described by the curve

$$\Lambda_f := \{(x_1, f(x_1)) : x_1 \in \mathbb{R}\}$$

with a periodic function f of period 2π. If nothing else is said we always assume that $f \in C^2(\mathbb{R})$. Let

$$\Omega_f := \{x \in \mathbb{R}^2 : x_2 > f(x_1),\ x_1 \in \mathbb{R}\}$$

be filled with a material whose index of refraction (or wave number) k is a positive constant, where $k = \omega c^{-1}(\mu\epsilon)^{1/2}$. Here ω is the angular frequency, c the speed of light, μ the magnetic permeability which is assumed to be 1 everywhere, and ϵ is the dielectric coefficient. Suppose that a plane wave given by

$$u^{in}(x) = \exp(i\alpha x_1 - i\beta x_2)$$

is incident on Λ_f from the top, where $\alpha = k\sin\theta$, $\beta = k\cos\theta$, and $\theta \in (-\pi/2, \pi/2)$ is the incident angle. Then the direct scattering problem is to find the scattered field $u \in C^2(\Omega_f) \cap C(\overline{\Omega}_f)$ such that

$$\Delta u + k^2 u = 0 \quad \text{in} \quad \Omega_f, \quad u = -u^{in} \quad \text{on} \quad \Lambda_f, \tag{2.1}$$

and (as the incident wave) u is assumed to be α-quasiperiodic:

$$u(x_1 + 2\pi, x_2) = \exp(2\pi i\alpha) u(x_1, x_2). \tag{2.2}$$

Moreover, we require that u satisfies a radiation (or outgoing wave) condition, i.e., u is composed of bounded outgoing plane waves:

$$u(x) = \sum_{n\in\mathbb{Z}} A_n \exp\{i(n+\alpha)x_1 + i\beta_n x_2)\}, \tag{2.3}$$

with $\beta_n := (k^2 - (n+\alpha)^2)^{1/2}$ for $|n+\alpha| \le k$, $\beta_n := i((n+\alpha)^2 - k^2)^{1/2}$ for $|n+\alpha| > k$ and the Rayleigh coefficients $A_n \in \mathbb{C}$. We further exclude resonances by assuming $\beta_n \neq 0$ for all $n \in \mathbb{Z}$ throughout the paper. Then the sum over the finite index set

$$\mathcal{U} := \{n \in \mathbb{Z} : |n+\alpha| < k\},$$

i.e. $\beta_n > 0$ for $n \in \mathcal{U}$, corresponds to the propagating modes of the scattered field, whereas the terms in (2.3) for $n \in \mathbb{Z}\setminus\mathcal{U}$ represent evanescent (exponentially decaying) waves. The optical efficiencies of the grating are defined by

$$e_n := (\beta_n/\beta)|A_n|^2, \; n \in \mathcal{U},$$

which is the ratio of the energy of the nth propagating mode to the energy of the incident wave.

The existence of a unique solution to the Dirichlet problem (2.1)–(2.3) is established by integral equation methods or variational methods (see, e.g., [12]), and the result may be generalized to arbitrary Lipschitz profiles [9]. Our goal in this paper is to study the inverse problem of profile reconstruction. More precisely, given the incident wave u^{in} and $b > \|f\|_{C(\mathbb{R})}$, we introduce the 'output' operator

$$A : f \to u(x_1, b),$$

which maps the profile function f onto the trace of the scattered field on the line $x_2 = b$. In terms of this operator, given the exact scattered field on $x_2 = b$ (or, equivalently, the Rayleigh coefficients A_n for all $n \in \mathbb{Z}$), the inverse problem just consists in solving the nonlinear and ill-posed equation

$$A(f) = u_b := u(x_1, b) \tag{2.4}$$

for the unknown profile function f. Hence it is quite natural to apply regularization methods to this equation.

Note that in problem (2.4) the knowledge of all modes of the scattered waves is required. From the practical point of view this is not quite satisfactory since one is not able to measure the evanescent waves far away from the grating structure. In our numerical implementation we therefore consider the following more practical reconstruction problem:

Given the Rayleigh coefficients A_n or the efficiencies e_n for $u \in \mathcal{U}$, i.e. for the propagating modes, possibly for several wave numbers and/or incident angles, determine a finite section of the Fourier series of the profile function f.

However, so far we are only able to prove some convergence results for the regularization methods applied to problem (2.4).

3 Tikhonov regularization

To deal with the ill-posedness for a stable profile reconstruction, a regularized version of (2.4) should be considered, e.g., the Tikhonov regularization. In the following, we choose $\mathcal{M}$ to be a set of 2π-periodic functions $f \in C^2(\mathbb{R})$, which is compact with respect to the convergence in the space of 2π-periodic C^1-functions. We further select b such that $b > \sup\{\|f\|_{C(\mathbb{R})} : f \in \mathcal{M}\}$ and consider the Tikhonov functional

$$F(f;\gamma) := \|Af - u_b\|^2 + \gamma\|f\|^2. \tag{3.1}$$

Here u_b is a measured scattered field on $x_2 = b$, $\|\cdot\|$ denotes the norm in the (complex) Hilbert space $X = L^2(0, 2\pi)$, and $\gamma > 0$ is the regularization parameter. It follows from the compactness of $\mathcal{M}$ and the fact that the output operator $A : \mathcal{M} \to X$ is continuous with respect to the convergence in $C^1(\mathbb{R})$ (see [12], Thm. 9) that for any $\gamma > 0$ there exists a minimizer $f_\gamma \in \mathcal{M}$ of (3.1), i.e.,

$$F(f_\gamma;\gamma) = \inf\{F(f;\gamma) : f \in \mathcal{M}\}.$$

Now let $\delta > 0$, and let $u_b^\delta \in X$ be a measured scattered field with noise level $\leq \delta^{1/2}$, i.e.,

$$\|u_b - u_b^\delta\|^2 \leq \delta, \tag{3.2}$$

where u_b is the exact pattern of the scattered field for some profile function $f_0 \in \mathcal{M}$:

$$Af_0 = u_b. \tag{3.3}$$

To approximate the reconstruction problem (3.3), we consider the Tikhonov functional (3.1) with u_b replaced by u_b^δ and choose the regularization parameter $\gamma := \delta$ following the strategy proposed in [6]:

$$F(f;\delta) := \|Af - u_b^\delta\|^2 + \delta\|f\|^2. \tag{3.4}$$

Let $f_\delta \in \mathcal{M}$ be a minimizer of (3.4). Using again the compactness of $\mathcal{M}$ and the continuity property of A mentioned above, one easily obtains the following result.

Proposition 3.1 *Let u_b be the exact output of the scattered field on $x_2 = b$ which corresponds to some profile function $f_0 \in \mathcal{M}$, and for any $\delta > 0$ let f_δ be a minimizer of the functional* (3.4). *Then for $\delta \to 0$ there exists a convergent subsequence $f_\delta \to f^*$, where the limit point $f^* \in \mathcal{M}$ represents a profile function with $Af^* = u_b$. Under the additional assumption that problem* (3.3) *is uniquely solvable, the total sequence (f_δ) converges to f_0.*

Proof. We have $Af_\delta \to Af^*$ in X. Furthermore, (3.2) and (3.3) imply the estimate

$$\begin{aligned} \|Af_\delta - Af_0\|^2 &\leq 2(\|Af_\delta - u_b^\delta\|^2 + \|u_b^\delta - u_b\|^2) \\ &\leq 2\delta + 2\min_{f\in\mathcal{M}}\{\|Af - u_b^\delta\|^2 + \delta\|f\|^2\} \\ &\leq 2\delta + 2(\|Af_0 - u_b^\delta\|^2 + \delta\|f_0\|^2) \leq C\delta, \end{aligned} \tag{3.5}$$

where C only depends on $\mathcal{M}$. Hence, $Af^* = Af_0 = u_b$. ∎

Remark 3.1 Problem (3.3) is uniquely solvable if the wavenumber k is sufficiently small (see [4],[10]). In the general case we can try to achieve uniqueness of problem (3.3) and more accurate reconstructions by using more incident waves $u_j^{in} (j = 1, ..., n)$ with different wavelengths and/or incident angles. In fact, it was proved in [10] that the grating profile is uniquely determined by a finite number of wave numbers if some a priori information on the amplitude of the periodic structure is available. For the Tikhonov regularization of (3.3) we then have to replace the cost functional (3.4) by a corresponding sum over j.

Remark 3.2 The above result may be extended to more general admissible sets of profile curves. Let $\mathcal{M}$ be a set of 2π-periodic Lipschitz functions, which is compact with respect to the convergence in $C(\mathbb{R})$. Then Proposition 3.1 carries over to this case since $f_n \to f$ in $C(\mathbb{R})$ implies $Af_n \to Af$ in X (see [9], Thm. 2.1).

Applying the stability result of [4], we can derive a convergence rate for the Tikhonov regularization of (3.3) when the wave number k is sufficiently small and an appropriate admissible set of smooth profiles with fixed endpoints is chosen. Given κ, $0 < \kappa \leq 1$ and $a \in \mathbb{R}$, let $\mathcal{M}$ be a set of 2π-periodic functions, which is bounded in the norm of $C^{3,\kappa}(\mathbb{R})$ and such that $f(0) = f(2\pi) = a$ for all $f \in \mathcal{M}$. Retaining the notation of Proposition 3.1, we are now in a position to prove the following theorem.

Theorem 3.1 *Assume that* $0 < k < 1/2\pi$. *Then*

$$\|f_\delta - f_0\|_{C(\mathbb{R})} \leq C/|\log\log(1/\delta)|, \tag{3.6}$$

where C *only depends on* $\mathcal{M}$.

Proof. Choose b_1 such that $b_1 > b > \sup\{\|f\|_{C(\mathbb{R})} : f \in \mathcal{M}\}$, and let A_1 be the output operator mapping the profile function onto the trace of the scattered field on $x_2 = b_1$. Then we have the stability estimate

$$\|f_\delta - f_0\|_{C(\mathbb{R})} \leq C/|\log\log(1/\|A_1 f_\delta - A_1 f_0\|_{H^1})|, \tag{3.7}$$

where C only depends on $\mathcal{M}$ and H^1 stands for the α-quasiperiodic Sobolev space of order 1. This follows from Theorem 2.1 in [4] after performing a suitable shift in x_2-direction.

Moreover, using the corresponding Rayleigh expansions (2.3) of the solutions u_0 and u_δ to the forward problem in Ω_{f_0} and Ω_{f_δ}, respectively, and the orthogonality of the functions $\exp(inx_1)$ in X, we obtain the elementary estimate

$$\|A_1 f_\delta - A_1 f_0\|_{H^1} \leq \|Af_\delta - Af_0\|, \tag{3.8}$$

with a constant c only depending on b and b_1. Combining (3.7), (3.8) and (3.5) then gives the desired bound (3.6). ■

Using local stability estimates (see [3] for smooth profiles and [8] for polygonal profiles), the double-log estimate (3.6) can be improved to a Lipschitz type estimate. However, this requires rather strong a priori assumptions on the admissible set $\mathcal{M}$.

4 An optimization method

We want to apply a method developed by Kirsch and Kress for the case of acoustic waves and bounded impenetrable obstacles; see [14] and the detailed presentation in [7]. Assume that we have the a priori information about our inverse periodic diffraction problem (2.4) that, without loss of generality, the unknown profile Λ_f lies above the line $x_2 = 0$ and below $x_2 = b$. We try to represent the scattered field as a single layer potential

$$u(x) = \int_0^{2\pi} \varphi(t) G(x_1, x_2, t, 0)\, dt \tag{4.1}$$

with an unknown density function $\varphi \in X = L^2(0,2\pi)$ and the free space quasiperiodic Green function (cf., e.g., [12])

$$G(x,y) = \frac{i}{2\pi} \sum_{n\in\mathbb{Z}} \frac{1}{\beta_n} \exp(i(n+\alpha)(x_1-y_1) + i\beta_n|x_2-y_2|),\ x \neq y. \tag{4.2}$$

The function (4.2) is well defined since we assumed $\beta_n \neq 0$ for all $n \in \mathbb{Z}$. For fixed f, introduce the linear operators $T, S_f : X \to X$ by

$$\begin{aligned} T\varphi(x_1) &= \int_0^{2\pi} \varphi(t) G(x_1, b, t, 0)dt, \\ S_f\varphi(x_1) &= \int_0^{2\pi} \varphi(t) G(x_1, f(x_1), t, 0)dt. \end{aligned} \tag{4.3}$$

Note that $T\varphi$ approximates the output Af of the scattered field u on $x_2 = b$, whereas $S_f\varphi$ (which is nonlinear with respect to f) represents an approximation of u on the profile Λ_f. Here and in the following we identify the (α-quasiperiodic) space $L^2(\Lambda_f)$ with X via

$$\|v \circ f\|_X = (\int_0^{2\pi} |v(f(x_1))|^2 dx_1)^{1/2}, v \in L^2(\Lambda_f),$$

which is a uniformly equivalent norm when f varies in a set of profile functions with uniformly bounded $C^{0,1}$ norm. If φ is given as a Fourier series

$$\varphi(t) = \sum_{n\in\mathbb{Z}} \varphi_n \exp(i(\alpha+n)t) \in X,\ \varphi_n \in \mathbb{C},$$

then from (4.2) and (4.3) we obtain

$$\begin{aligned} T\varphi(t) &= i \sum_{n\in\mathbb{Z}} \varphi_n \beta_n^{-1} \exp(i(\alpha+n)t + i\beta_n b), \\ S_f\varphi(t) &= i \sum_{n\in\mathbb{Z}} \varphi_n \beta_n^{-1} \exp(i(\alpha+n)t + i\beta_n f(t)). \end{aligned} \tag{4.4}$$

Because of $|\beta_n| \sim |n|$ as $n \to \infty$ and our a priori assumption on Λ_f, the series in (4.4) are convergent in any α-quasiperiodic Sobolev norm. Moreover, it can be easily checked that $T : X \to X$ is an injective compact operator with dense range and with the exponentially decreasing singular values $|\beta_n^{-1} \exp(i\beta_n b)|$. Hence, given the output u_b of the scattered field, the determination of the density φ from u_b by solving the first kind equation $T\varphi = u_b$ is a severely ill-posed problem.

We may solve its Tikhonov regularized version

$$\gamma\varphi + T^*T\varphi = T^*u_b, \tag{4.5}$$

with regularization parameter $\gamma > 0$. Given the solution $\varphi_\gamma \in X$ of (4.5) and the corresponding approximation u_γ of the scattered field, we can then seek the profile Λ_f of the grating by minimizing the defect

$$\|u^{in} + u_\gamma\|_{L^2(\Lambda_f)},\ f \in \mathcal{M}, \tag{4.6}$$

over a class of admissible curves Λ_f. In the following we will choose $\mathcal{M}$ to be a compact set (with respect to the $C^{1,\delta}$ norm, $0 < \delta \leq 1$) of all 2π-periodic C^2 functions such that

$$0 < c \leq \inf\{\|f\|_{C(\mathbb{R})} : f \in \mathcal{M}\}, \quad \sup\{\|f\|_{C(\mathbb{R})} : f \in \mathcal{M}\} \leq d < b.$$

For a reformulation of the inverse diffraction problem (2.4) as an optimization problem, we now combine the minimization of the Tikhonov functional for (4.5) and the defect minimization (4.6) into the following cost functional:

$$F(\varphi, f; \gamma) := \|T\varphi - u_b\|^2 + \gamma\|\varphi\|^2 + \rho\|u^{in} \circ f + S_f\varphi\|^2. \tag{4.7}$$

Here, $\gamma > 0$ is again the regularization parameter and $\rho > 0$ denotes a coupling parameter which has to be chosen appropriately for the numerical implementation. The justification of the ansatz (4.1) and the choice of the cost functional (4.7) is given by the following lemma.

Lemma 4.1 *For any profile Λ_f, $f \in \mathcal{M}$, $S_f : X \to L^2(\Lambda_f)$ is an injective compact operator with dense range.*

The proof is given in [13], Lemma 3.2. Our method now consists in solving the following optimization problem.

(**OP**): Find $\varphi \in X$ and $f \in \mathcal{M}$ such that

$$F(\varphi, f; \gamma) = m(\gamma) := \inf\{F(\psi, g; \gamma) : \psi \in X, g \in \mathcal{M}\}.$$

The existence of a minimizer is guaranteed by the following theorem.

Theorem 4.1 *For each $\gamma > 0$ the problem* (OP) *has a solution.*

Here we need not assume that u_b is an exact output of the scattered field. The proof is analogous to that of Theorem 5.20 in [7]. Applying the integral equation method of [13] and the arguments used in the proof of Theorems 5.21 and 5.22 in [7], we obtain the following convergence result.

Theorem 4.2 *Let u_b be the exact pattern of the scattered field u on $x_2 = b$ which corresponds to some profile curve $f \in \mathcal{M}$. Then we have:*

(i) $\lim_{\gamma\to 0} m(\gamma) = 0$.

(ii) *Let (γ_n) be a null sequence and let (φ_n, f_n) be a corresponding sequence of solutions to* (OP) *with regularization parameter γ_n. Then there exists a convergent subsequence of (f_n), and every limit point f^* of (f_n) represents a profile function such that the total field $u^{in} + u$ vanishes on Λ_{f^*}.*

If we have the a priori information that the inverse problem (2.4) is uniqely solvable (e.g., for sufficiently small wave number or height of the grating, see [10]), we obtain convergence of the total sequence (f_n) to f. As in Remark 3.2 we can achieve uniqeness and more accurate reconstructions by replacing the cost functional (4.7) by a sum corresponding to several incident waves.

Remark 4.1 The above results on the problem (OP) can be generalized to admissible sets of Lipschitz profiles. Let f and f_n ($n \in \mathbb{N}$) be 2π-periodic Lipschitz functions, and define the convergence $f_n \to f$ in the sense that

$$\|f_n - f\|_{C(\mathbb{R})} \longrightarrow 0 \quad \text{and} \quad \|f_n\|_{C^{0,1}(\mathbb{R})} \le c \quad \text{as} \quad n \to \infty. \tag{4.8}$$

Let $\mathcal{M}$ be a set of 2π-periodic Lipschitz functions, which is compact with respect to the convergence defined in (4.8). Then Theorems 4.2 and 4.3 carry over to this case; see [9] for the proof which is based on the variational approach to the direct problem (2.1)–(2.3) rather than on integral equation methods.

5 The reconstruction algorithm

We now discuss the implementation of our optimization method for the reconstruction problem introduced at the end of Section 2. In this problem, given the Rayleigh coefficients $A_n, n \in \mathcal{U}$, for the propagating modes, we approximate the unknown profile function f as a truncated Fourier series

$$f(t) = \sum_{|m| \le M} c_m \exp(imt), \tag{5.1}$$

where $c_{-m} = \overline{c_m}$ for all indices m. Moreover, the unknown density ϕ in (4.1) is also sought as a trigonometric polynomial

$$\phi(t) = \sum_{|n| \le N} a_n \exp(int).$$

Introducing the vectors

$$y = (a, c), \quad a = (a_n) \in \mathbb{C}^{2N+1}, \quad c = (c_m) \in \mathbb{C}^{2M+1}$$

and replacing the scattered field u_b on the line $x_2 = b$ by the 'far field'

$$u_\infty(t) := \sum_{n \in \mathcal{U}} A_n \exp\{i(n+\alpha)t + i\beta_n b\},$$

the cost functional (4.7) then takes the form

$$\|T\varphi - u_\infty\|^2 + \gamma\|\varphi\|^2 + \rho\|u^{in} \circ f + S_f\varphi\|^2$$

$$= 2\pi \sum_{|n| \le N} (|g_n(a)|^2 + \gamma|a_n|^2) + \rho \int_0^{2\pi} |h(y;t)|^2 dt, \tag{5.2}$$

where

$$\begin{aligned} g_n(a) &= i\beta_n^{-1} a_n - A_n\,, \; n \in \mathcal{U}; \quad g_n(a) = i\beta_n^{-1} \exp(i\beta_n b)\, a_n\,, \; n \notin \mathcal{U}; \\ h(y;t) &= \exp\Big(- i\beta \sum_{|m| \le M} c_m \exp(imt)\Big) \\ &\quad + \sum_{|n| \le N} i\beta_n^{-1} a_n \exp\Big(int + i\beta_n \sum_{|m| \le M} c_m \exp(imt)\Big). \end{aligned} \tag{5.3}$$

The integral in (5.2) is discretized using the trapezoidal rule for 2π-periodic functions:

$$\int_0^{2\pi} |h(y;t)|^2 dt \;\approx\; (2\pi/K) \sum_{j=1}^{K} |h(y;2\pi j/K)|^2.$$

The problem (OP) is then replaced by the finite dimensional nonlinear least squares problem

$$\min \left\{ \|\mathcal{F}(y)\|^2_{\mathbb{C}^{4N+K+2}} \,:\, y \in \mathbb{C}^{2(N+M+1)} \right\}, \tag{5.4}$$

where the first $2N+1$ components of $\mathcal{F}$ are constant multiples of the linear functions $g_n(a)$ defined in (5.3), the next $2N+1$ components are equal to $(2\pi\gamma)^{1/2}a_n$, and the last K components are given by

$$\mathcal{F}_{j+4N+2}(y) = (2\pi\rho/K)^{1/2}\; h(y;2\pi j/K), \quad j = 1, ..., K. \tag{5.5}$$

In the Levenberg–Marquardt method (see, e.g., [15]), the solution of the nonlinear problem (5.4) is obtained iteratively by solving the linear least squares problem

$$\min \left\{ \|\mathcal{F}'(y)p + \mathcal{F}(y)\|^2_{\mathbb{C}^{4N+K+2}} + \lambda I \|p\|^2_{\mathbb{C}^{2(N+M+1)}} \,:\, p \in \mathbb{C}^{2(N+M+1)} \right\} \tag{5.6}$$

at each iteration step. Here the current iterate is sought in the form $y+p$ where y denotes the preceding iterate, $\mathcal{F}'(y)$ stands for the Jacobian matrix of $\mathcal{F}$ evaluated at y, and the parameter $\lambda \geq 0$ is suitably chosen (note that $\lambda = 0$ corresponds to the Gauss–Newton method). The normal equations for (5.6) to be solved at each iteration are

$$(\mathcal{F}'(y)^* \mathcal{F}'(y) + \lambda I)p \;=\; -\mathcal{F}'(y)^* \mathcal{F}(y),$$

where the star designates the adjoint matrix and I is the unit matrix of order $2(N+M+1)$. The entries of $\mathcal{F}'(y)$ can be obtained immediately from (5.3) and (5.5). Note that we have, in particular, the decomposition

$$\mathcal{F}'(y)^* \mathcal{F}'(y) \;=\; \begin{pmatrix} \mathcal{A}+\mathcal{D} & \mathcal{C} \\ \mathcal{C}^* & \mathcal{B} \end{pmatrix},$$

where $\mathcal{D}$ is the diagonal matrix of order $2N+1$ with entries $2\pi(|\beta_n^{-1}\exp(i\beta_n b)|^2 + \gamma)$, $|n| \leq N$, independent of y, whereas the entries of $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$ are expressible in terms of the partial derivatives of the functions $h(\,\cdot\,;2\pi j/K)$, $j = 1, ..., K$, at $y = (a,c)$.

To implement the reconstruction algorithm for nonsmooth profiles, the unknown profile function should rather be sought as a spline (e.g., a piecewise linear function) with fixed equidistant knots or with free knots on the interval $[0, 2\pi]$. In that case the integrals occurring in the last term of (5.2) can be calculated analytically.

6 Numerical results

Here we present the results of numerical experiments using our method with synthetic data in the case of a smooth profile function $f(t)$ given as a trigonometric polynomial (5.1). We performed numerical experiments for the following two profile functions, chosen as in the examples discussed in [5] and [11] :

$$f(t) = h\cos(t) + c_0\,, \tag{6.1}$$

$$f(t) = h(\cos(t) + \cos(2t) + \cos(3t)) + c_0 \,. \tag{6.2}$$

We chose $c_0 = 2$ and $h > 0$ small enough so that $f(t) > 0$ for $t \in [0, 2\pi]$.

The far field data, i.e., the Rayleigh coefficients of the propagating modes, were generated solving the direct problem by the analytic continuation method presented in [5] and [11]. In the inverse computation we applied the optimization method described in Section 5 to reconstruct the target profiles (6.1) and (6.2). The set of admissible profiles was taken to coincide with the family of Fourier gratings with three and seven modes, i.e. $M = 1$ and $M = 3$, respectively, in (5.1). Usually, we used the far field data for a number n_I of different incident waves with characteristics (l_j, θ_j), $j = 1, ..., n_I$. Here an incident plane wave is characterized by the pair (l, θ), where $l := 1/k$, k is the wave number, and θ denotes the incident angle. Recall that γ is the regularization parameter and ρ the weight of the last term in the cost functional. The number of Gauss-Newton or Levenberg-Marquardt iterations is denoted by n_{it}.

We first considered profile curves of the form (6.1) and incident waves of the following characteristics:

1: $n_I = 1, \quad (\ell, \theta) = (.55, 0),$
2: $n_I = 1, \quad (\ell, \theta) = (.22, 0),$
3: $n_I = 2, \quad (\ell, \theta) = (.22, 0.5),\ (.22, -0.5),$
4: $n_I = 1, \quad (\ell, \theta) = (.22, 0.5).$

With respect to the three values $h = 0.10\pi,\ 0.15\pi,\ 0.20\pi$ we performed three series **A, B, C** of experiments with the incident waves **1**–**4** in each case. The number of iterations was varied from 10 to 100 if necessary. Because of the unsymmetry of data, we took $\gamma = 1,\ \rho = 10^{-1}$ and $\gamma = 10^2,\ \rho = 1$ in experiments **B4** and **B4**, respectively, whereas the choice $\gamma = 10^{-8},\ \rho = 10^{-1}$ was satisfactory in all other cases. The numerical results are given in the following three tables:

	target	initial	**A1**	**A2**	**A3**	**A4**
c_{-1}	0.1570796	0.0	0.157075	0.157077	0.1570494	0.1571
c_0	2.000000	2.0	2.00000	2.000004	2.00001	2.0007
c_1	0.1570796	0.0	0.157075	0.157080	0.1570498	0.1562

	target	initial	**B1**	**B2**	**B3**	**B4**
c_{-1}	0.235619	0.1	0.2355	0.23559	0.23507	0.2344
c_0	2.000000	2.0	2.00001	1.9999996	2.0003	2.007
c_1	0.235619	0.1	0.2355	0.235617	0.23506	0.2292

	target	initial	**C1**	**C2**	**C3**	**C4**
c_{-1}	0.3141	0.1	0.3136	0.3144	0.311	0.2839
c_0	2.000000	2.0	2.00003	2.0005	2.002	2.03
c_1	0.3141	0.1	0.3136	0.3140	0.311	0.2835

Table 1: Experiments in the case (6.1)

In the case of profile functions of the form (6.2) we only considered 'symmetrical data', i.e., the profile is symmetrically illuminated. Then the computation requires almost no regularization, and the computed coefficients turn out to be symmetrical in the sense that $c_{-m} \approx c_m$. Moreover, we took $n_{it} = 50$ and $\gamma = 10^{-8}$, $\rho = 10^{-1}$.

In a first series of experiments we chose $h = 0.05\pi$, which is very close to the choice $h = 0.045\pi$ in [11]. In the experiments **1**, **2**, **3** we fixed $l = 0.44$ and varied the incoming wave with respect to its incidencent angle θ:

1: $n_I = 2, \quad \theta = 0.5, -0.5,$
2: $n_I = 5, \quad \theta = 1., 0.5, 0., -0.5, -1$
3: $n_I = 11, \quad \theta = 1.3, 1., 0.8, 0.5, 0.25, 0., -0.25, -0.5, -0.8, -1., -1.3$

Then we varied both the wave number and incident angle:

4: $n_I = 4, \quad (\ell, \theta) = (.44, .5), (.44, -.5), (.54, .5), (.54, -.5)$
5: $n_I = 6, \quad (\ell, \theta) = (.44, .5), (.44, -.5), (.54, .5), (.54, -.5), (.64, .5), (.64, -.5)$
6: $n_I = 15, \quad (\ell, \theta) = (.44, 1.), (.44, .5), (.44, 0.), (.44, -.5), (.44, -1.), (.59, 1.), (.59, .5), (.59, 0.), (.59, -.5), (.59, -1.), (.74, 1.), (.74, .5), (.74, 0.), (.74, -.5), (.74, -1.)$

Finally, we fixed $\theta = 0$ and changed only the wave number:

7: $n_I = 15, \quad \ell = .44, .46, .49, .51, .54, .56, .59, .62, .64, .67, .69, .71, .74, .77, .79$

In the following table the computed real parts of the coefficients c_m, $m = 0, .., 3$, are given. The imaginary parts turned out to be at least one order in magnitude smaller than the real parts.

c	target	initial	**1**	**2**	**3**	**4**	**5**	**6**	**7**
0	2.0000	1.9	2.0138	2.0078	2.0063	2.016	2.018	2.011	2.023
1	0.0785	0.13	0.0865	0.0813	0.0804	0.0860	0.0861	0.0824	0.0948
2	0.0785	0.0	0.0664	0.0750	0.0764	0.0677	0.0681	0.0739	0.0853
3	0.0785	0.0	0.0590	0.0666	0.0683	0.0517	0.0468	0.0608	-0.0047

Table 2: Case (6.2) for $h = 0.05\pi$

In a second series of experiments we chose $h = 0,005\pi$ and the following incident waves:

8: $n_I = 2, \quad (\ell, \theta) = (.44, .5), (.44, -.5)$
9: $n_I = 4, \quad (\ell, \theta) = (.44, .5), (.44, -.5), (.54, .5), (.54, -.5)$
10: $n_I = 6, \quad (\ell, \theta) = (.44, .5), (.44, -.5), (.54, .5), (.54, -.5), (.64, .5), (.64, -.5)$

Here, much better results were obtained than in the preceding examples:

c	target	initial	**8**	**9**	**10**
0	2.00000	1.9	2.000003	2.000005	2.000006
1	0.007853	0.0	0.007857	0.007855	0.007854
2	0.007853	0.0	0.0078270	0.0078279	0.0078285
3	0.007853	0.0	0.00781	0.00778	0.00776

Table 3: Case (6.2) for $h = 0.005\pi$

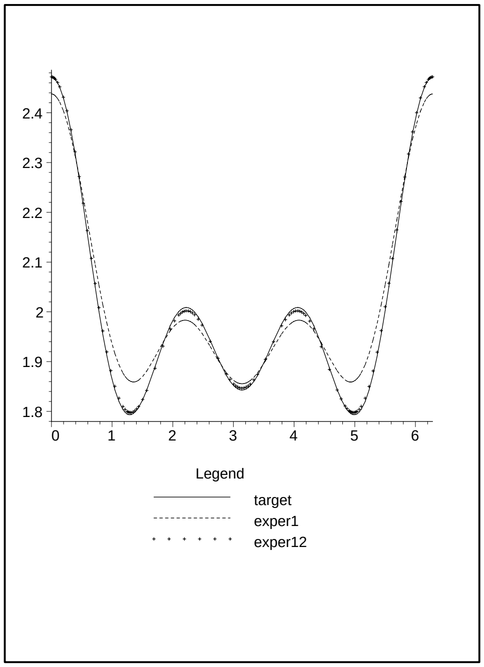

Figure 1: $|m| \leq 3$

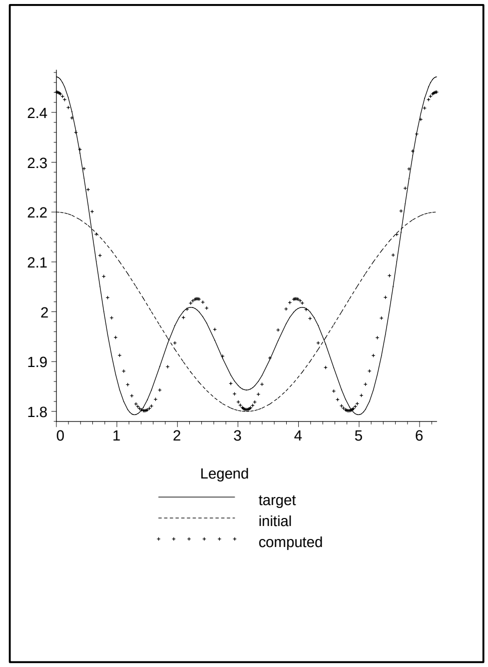

Figure 2: $|m| \leq 5$

Finally, we considered far field data of higher frequency:

11: $h = 0.005\pi, \quad n_I = 1, \quad (\ell, \theta) = (0.22, 0.)$
12: $h = 0.05\pi, \quad n_I = 1, \quad (\ell, \theta) = (0.22, 0.)$

c	target	initial	**11**	target	initial	**12**
0	2.000000	1.9	2.000001	2.00000	2.1	2.0008
1	0.00785398	0.0	0.0078541	0.07853	0.0	0.0804
2	0.00785398	0.0	0.00785399	0.07853	0.0	0.0793
3	0.00785398	0.0	0.00785397	0.07853	0.0	0.0759

Table 4: Case (6.2) for $\ell = 0.22$

In Figure 1 the results of experiments 1 (cf. Table 2) and 12 (cf. Table 4) are plotted compared with the target profile. Figure 2 shows the profile of experiment 12 computed using the weaker a priori information $|m| \leq 5$ in comparison with the respective initial guess and target profile.

As a result of the computations, we obtained satisfactory approximations of the target parameters, rather independent on the initial guess. We observed the following:

1) The performance of the algorithm depends on the amplitude of the target profile and on the character of the far field data. The reconstruction of the target is rather good if the profile is flat enough. It becomes worse if the steepness of the profile increases. Moreover, higher frequency data lead to a more accurate reconstruction than in the lower frequency case.

2) If one uses data from a symmetrical illumination of the profile, then a regularization is

not needed. On the other hand, in the unsymmetrical case a strong regularization might be necessary to produce satisfactory numerical results.

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