

Nonlinearity parameter imaging in the frequency domain

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Abstract

Nonlinearity parameter tomography leads to the problem of identifying a coefficient in a nonlinear wave equation (such as the Westervelt equation) modelling ultrasound propagation. In this paper we transfer this into frequency domain, where the Westervelt equation gets replaced by a coupled system of Helmholtz equations with quadratic nonlinearities. For the case of the to-be-determined nonlinearity coefficient being a characteristic function of an unknown not necessarily connected domain D , we devise and test a reconstruction algorithm based on weighted point source approximations combined with Newton's method. In an abstract setting, convergence of a regularised Newton type method for this inverse problem is proven by verifying a range invariance condition for the forward operator and establishing injectivity of its linearisation.

key words: nonlinearity parameter tomography, multi-harmonic expansion, Westervelt equation, Helmholtz equation, extended sources, point sources, Newton's method, range invariance condition

1 Introduction

Nonlinearity parameter tomography [7, 9, 10, 21, 36, 41, 42, 43], is a technique for enhanced ultrasound imaging and amounts to identifying the spatially varying coefficient $\eta = \eta(x)$ in the Westervelt equation

$$p_{tt} - c^2 \Delta p - b \Delta p = \eta(p)_{tt} + h \text{ in } (0, T) \times \Omega, \quad (1)$$

from observations of the pressure

$$y(x, t) = p(x, t), (x, t) \in \Sigma \times (0, T) \quad (2)$$

on some manifold Σ immersed in the acoustic domain Ω or attached to its boundary $\Sigma \subseteq \bar{\Omega}$; see [22, 26, 27, 28] and the references therein. In (1) p is the acoustic pressure, c is the speed of sound, b is the nonlinearity parameter, h is the source term, and η is the nonlinearity coefficient.

is the excitation and the constants $b > 0$ are the speed and diffusivity of sound, respectively. rep Y (19)

While uniqueness from the Dirichlet-to-Neumann operator has been established in [2], our aim here is to reconstruct η from the single boundary measurement (2) like in [26, 27, 28].

Here we will consider this problem in the frequency domain, inspired by the concept of harmonic imaging [4, 40, 41]. Due to the quadratic nonlinearity appearing in the PDE, this is not directly possible by the usual approach of taking the Fourier transform in time. Rather, the idea is to use a multi-harmonic ansatz [24] as follows.

Assuming periodic excitations of the specific form $h(x)\hat{h}(t) = \sum_{k=1}^{\infty} \hat{h}_k(x)e^{ik\omega t}$ (for some fixed frequency ω and $\hat{h} \in L^2(\Omega; \mathbb{C})$) and inserting a multi-harmonic expansion for a time periodic solution of (1) (that due to periodicity of h can be proven to exist and be unique) $p(x, t) = \sum_{k=1}^{\infty} \hat{p}_k(x)e^{ik\omega t}$ into (1), yields the infinite system of coupled linear Helmholtz type PDEs

$$\begin{aligned} m = 1 : \quad & -\omega^2 \hat{p}_1 - (c^2 + i\omega b)\hat{p}_1 = \hat{h} - \frac{\eta}{2}\omega^2 \sum_{k=2}^{\infty} \overline{\hat{p}_{\frac{k-1}{2}}} \hat{p}_{\frac{k+1}{2}} \\ m \in \{2, \dots, M\} : & \omega^2 m^2 \hat{p}_m - (c^2 + i\omega m b)\hat{p}_m \\ & = -\frac{\eta}{4}\omega^2 m^2 \sum_{k=1}^{m-1} \hat{p}_k \hat{p}_{m-k} + 2 \sum_{k=m+2, 2}^{\infty} \overline{\hat{p}_{\frac{k-m}{2}}} \hat{p}_{\frac{k+m}{2}} . \end{aligned} \quad (3)$$

This is obtained by using the Cauchy product formula for two series $\sum_{j=0}^{\infty} b_j = \sum_{k=0}^{\infty} \sum_{l=0}^k a_l b_{k-l}$ and relying on linear independence of the functions $t \mapsto \exp(i\omega t)$, that is, comparing coefficients leading to the same multiple of the fundamental frequency ω . Here the notation $\sum_{k=m+2, 2}^{\infty}$ means that the index takes steps of length two and thus runs over $m+2, m+4, m+6, \dots$; analogously for $\sum_{k=3, 2}^{\infty}$. The equivalence (3) to (1) holds with $M = \infty$, as shown in [24]. The fact that in place of single Helmholtz equation we have a system (in theory even an infinite one) reveals that nonlinearity actually helps the identifiability. This can be explained by the additional information available due to the appearance of several higher harmonics (similarly to several components arising in the asymptotic expansion in [30]). In practice the under-braced terms are often skipped and the expansion is only considered up to $M = 2$ or $M = 3$ (see [18, Chapter 5]). This is due to the fact that the strength of the signal in these higher harmonics decreases extremely quickly. In fact in our reconstructions, only two of them will be of effective use as the third harmonic only provides marginal improvement over the second one.

In our reconstructions in Section 2, we will focus on the case of a piecewise constant coefficient $\eta = \chi_D$ with a known constant η_0 and an unknown domain D that (??)

1 (upon skipping the under-braced terms) becomes

rep Y (2)

rep X p2, l.26

$$\begin{aligned} m = 1 : \quad & 4\hat{p}_1 + \kappa_1^2 \hat{p}_1 = \hat{h} \\ m \in \{2, \dots, M\} : \quad & \hat{p}_m + m^2 \kappa_m^2 \hat{p}_m = \frac{n_D}{4} \chi_D m^2 \kappa_m^2 \sum_{\ell=1}^{M-1} \hat{p}_\ell \hat{p}_{m-\ell}, \end{aligned} \quad (4)$$

2 where $\kappa = \sqrt{\frac{\omega}{c^2 + i\omega mb}}$ is the wave number. We do so for practical relevance (e.g., location p.2 (4)
 3 of contrast agents such as microbubbles on a homogeneous background) and for expected
 4 better identifiability as compared to a generation η (although counterexamples to
 5 uniqueness still exist cf., e.g., [3, 29], for the Helmholtz equation as opposed to the Laplace
 6 equation). Typically D will not necessarily be connected but consist of a union of con-
 7 nected components $D \stackrel{m}{=} \bigcup_{m=1}^M D_m$ that we will call inclusions or objects for obvious reasons.

8 Moreover, throughout this paper we assume the sound speed c to be known and con-
 9 stant. For results (in the time domain formulation (1)) on simultaneous identification of
 10 space dependent functions c and η , we refer to [28].

11 We will consider (3) on a smooth bounded domain $\Omega \subseteq \mathbb{R}^3$ with observations
 12 on a subset of $\partial\Omega$ and equip it with a boundary damping condition

$$\partial_\nu \hat{p}_m + (im\omega\beta + \gamma)\hat{p}_m = 0 \quad \text{on } \partial\Omega \quad (5)$$

13 with $\beta, \gamma \geq 0$ so that the parameter $(im\omega\beta + \gamma)$ quantifies the damping properties of the
 14 boundary – either for physical or computational purposes. In the latter sense, these rep Y (3)
 15 are direct translations to frequency domain zeroth and first order absorbing boundary
 16 conditions in time domain, see, e.g., the review articles [15, 17] and the references therein.
 17 Indeed, these boundary attenuation conditions even allow us to skip the interior damping
 18 and assume κ to be real valued, as has been shown in [23] in the time domain setting of
 19 (1). We will do so by working with a real valued wave number. In numerical tests of
 20 Section 2.

21 In the case where the observation manifold is contained in the boundary of the domain
 22 Ω , we can choose between writing the data (2) as Dirichlet trace $\hat{p}_m|_\Sigma$, impedance
 23 condition (5), with $g = -(im\kappa + \gamma)\hat{p}_m$, as Neumann trace

$$y_m = \hat{p}_m \quad \text{or} \quad g_m = \partial_\nu \hat{p}_m \quad \text{in } \Sigma, \quad m \in \{2, \dots, M\}. \quad (6)$$

24 In our numerical reconstructions we will also consider the practically relevant case of only
 25 partial data being available with $\Sigma \subseteq \partial\Omega$ being a strict subset. That according to the
 26 first line in (4) that does not contain the unknown D , observations on the fundamental
 27 harmonic y or g are not expected to carry essential information on D and are therefore
 28 neglected.

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2 A reconstruction method for piecewise constant η and numerical results

We first of all consider (4) for $M = 2$ and devise a reconstruction method based on the approach in [29]. While the algorithms described below work in both 2-d and 3-d, we confine the exposition and our numerical experiments to two space dimensions. In our numerical tests we will also study the question whether taking into account another harmonic $M = 3$ improves the results.

Having computed \hat{p} from the first equation in (??) with given excitations, the problem of determining η from the second equation in (??) reduces to an inverse source problem for the Helmholtz equation

$$4u + \tilde{\kappa}^2 u = \tilde{\kappa}^2 \eta \tilde{f} \quad \text{in } \Omega \quad (7)$$

where $u \in \hat{\mathcal{D}}_2$, $\tilde{\kappa} = \frac{2\omega}{c}$, $\tilde{f} = \frac{1}{4}\hat{p}_1$.

rep X p.4, l.1

In the case of a piecewise constant coefficient as considered here, (7) becomes

$$4u + \tilde{\kappa}^2 u = \tilde{\kappa}^2 \chi_D f \quad \text{in } \Omega. \quad (8)$$

with $f = \eta \tilde{f}$. There exists a large body of work on inverse source problems for the Helmholtz equation. Two particular examples for the case of extended sources as related to our setting are [22, 9]. We also point to, e.g., [1, 3, 6, 11, 13] for inverse source problems with multi frequency data; however these do not cover the important special case of restricting observations to higher harmonics of a single fundamental frequency.

We here intend to follow the approach from [12, 9]. Here, as an auxiliary problem, we will consider the Helmholtz equation with point sources

$$4u + \tilde{\kappa}^2 u = \sum_{k=1}^N \lambda_k \delta_{S_k} \quad \text{in } \Omega. \quad (9)$$

with δ distributions located at points S_k or more generally with a measure $\mu \in M(\Omega) = C_b(\bar{\Omega})^*$ as right hand side

$$4u + \tilde{\kappa}^2 u = \mu \quad \text{in } \Omega. \quad (10)$$

The PDEs (8), (9), (10) are equipped with impedance boundary conditions

$$\partial_\nu u + \tilde{\kappa} u = 0 \quad \text{on } \partial\Omega. \quad (11)$$

Results on well-posedness for the forward problems (7), (9), (11) can be found, e.g., in [35, Section VIII] and [38, Section 2].

An essential fact connecting (8) and (9) is that for any solution w of the homogeneous Helmholtz equation $4w + \tilde{\kappa}^2 w = 0$ on Ω , from Green's second identity, written in the form

$$\int_{\Omega} u (4w + \tilde{\kappa}^2 w) - w (4u + \tilde{\kappa}^2 u) \, dx = \int_{\partial\Omega} u (\partial_\nu w + \tilde{\kappa} w) - w (\partial_\nu u + \tilde{\kappa} u) \, ds$$

1 the following relations hold

$$\begin{aligned} & \int_{\partial\Omega} \partial_\nu u (\partial_\nu w + \tilde{\kappa} w) ds \\ & = -\tilde{\kappa} \int_{\partial\Omega} u (\partial_\nu w + \tilde{\kappa} w) ds = \begin{cases} i\tilde{\kappa} \int_D \tilde{\kappa}^2 f w dx & \text{for (8), (11)} \\ i\tilde{\kappa} \sum_{k=1}^n \lambda_k w(S_k) & \text{for (9), (11).} \end{cases} \end{aligned} \quad (12)$$

2 Combining this with a mean value identity for the Helmholtz equation

rep X p.4, (13)

$$\frac{1}{|B_r(x_0)|} \int_{B_r(x_0)} w dx = \Gamma_{\frac{d}{2}} + 1 \frac{J_{d/2}(\tilde{\kappa} r)}{(\tilde{\kappa} r/2)^{d/2}} w(x_0) \quad (13)$$

3 for any $r > 0$, and $x_0 \in \Omega$ such that $B_r(x_0) \subseteq \Omega$, and w solving $4w + \tilde{\kappa}^2 w = 0$ (see, e.g.,
4 [31] and the references therein), equivalence of (8), (9) in the case of constant background
5 f is obtained. In (13), $J_{d/2}$ is the Bessel function of the first kind viewed as an identity
6 of functionals acting on w , (13) reads (in our two dimensional setting $d = 2$) as

$$\begin{aligned} \chi_{B_r(x_0)} &= \lambda \delta_{x_0} \quad \text{on } \ker(4 + \tilde{\kappa}^2 \text{id}) \\ \text{where } \lambda &= \frac{2}{r\pi} \frac{J_1(\tilde{\kappa} r)}{\tilde{\kappa}} \end{aligned} \quad (14)$$

7 which makes the relation between inclusions as appearing in (8) with $f \equiv \text{const.}$ and point
8 sources as appearing in (9) obvious. Note that (13) remains valid in \mathbb{R}^d as a zero of
9 the Bessel function $J_{d/2}$, in which $\tilde{\kappa}^2$ is an eigenvalue of the Laplacian with homogeneous
10 Dirichlet boundary conditions on $\partial B_r(x_0)$, cf. [31, Section 3].

rep X p.5, Lm2

11 **Lemma 2.1** Assume that D can be represented as the union of n disjoint discs or balls.
12 Then there exist n points S_1, \dots, S_n and values $\lambda_1, \dots, \lambda_n$ such that for w solving (8) and
13 u_p solving (9) (both with boundary conditions (11)) the identity

$$\int_{\partial\Omega} \partial_\nu u_D (\partial_\nu w + \tilde{\kappa} w) ds = \int_{\partial\Omega} \partial_\nu u_p (\partial_\nu w + \tilde{\kappa} w) ds \quad \text{for all } w \in \ker(4 + \tilde{\kappa}^2 \text{id})$$

14 holds.

rep X p.5, l.2

15 The method from [29] uses a Padé approximation scheme (see [19], which was inspired
16 by [5]) for recovering point sources in the Laplace equation and a fixed point scheme
17 to extend this for finding point sources in the Helmholtz equation. This is proven
18 to converge in [29, Theorem 1] for sufficiently small wave numbers and the numerical
19 experiments there show that it works exceedingly well. However, in ultrasonics, $\tilde{\kappa}$
20 is large. Transition from the Laplace point source problem to the Helmholtz point source
21 problem therefore does not seem to be feasible in that situation. However, transition
22 from the Helmholtz point source problem (9) to the Helmholtz inclusion problem (8) is

rep Y (6)

¹Here the functional $\chi_{B_r(x_0)}$ is identified with its Riesz representer in the Hilbert space $L^2(\Omega)$.

still justified by Lemma 2.1, in case of circular or spherical inclusions and a constant background f .

In place of the Padé approximation algorithm in [29], we employ the primal-dual active point PDAP algorithm from [38], which we provide here for the convenience of the reader. It uses the forward operator $M(\Omega) \rightarrow L^2(\Sigma)$, $\mu \mapsto \partial u|_{\Sigma}$,² where u solves (10), (11) and its Banach space adjoint. The algorithm aims at solving the minimisation problem

$$\min_{\mu \in M(\Omega)} \frac{1}{2} k \partial_\nu u - g|_{L^2(\Sigma)}^2 + \theta k \mu|_{M(\Omega)} \quad \text{s.t. } u \text{ solves (10), (11)}$$

with some regularisation parameter $\theta > 0$ (whose value actually does not matter much, due to one-homogeneity of the regularisation functional), which in case of Σ being a discrete set can be shown to have a solution of the form $\mu = \sum_{k=1}^n \lambda_k \delta_{S_k}$ for some coefficients $\lambda_k \in \mathbb{R}$ and points $S_k \in \Omega$. The method can be motivated by gradient descent for this minimisation problem in a generalised sense of non-smooth convex optimisation. Starting from $\mu = 0$ the method first proposes a new source location $\hat{S}_1 \in \Omega$ corresponding to a maximum of the norm of the current dual variable $F^*(F\mu - g)$. The new point is added to the support of the current iterate. The algorithm as described in [38] also contains a point removal step, which we skip here, though. As a stopping criterion, a sufficient decrease (by a factor of 10^6 in our computations) of the primal-dual gap is used.

Algorithm PDAP:

For $i = 1, 2, 3, \dots$

1. Compute $\xi := F^*(F\mu - g)$; determine $\hat{S}^i \in \arg\max_{x \in \Omega} |\xi(x)|$

2. Set $(S_1, \dots, S_n) := \text{supp}(\mu) \cup \{\hat{S}^i\}$;

3. compute a minimiser $\lambda \in \mathbb{R}^n$ of $j(\lambda) := k F^P \sum_{k=1}^n \lambda_k \delta_{S_k} - g|_{L^2(\Sigma)}^2$

4. Set $\mu^{i+1} = \sum_{k=1}^n \lambda_k^i \delta_{S_k^i}$

This also yields the number n of point sources.

Combining this with the other elements from the method in [29], arrive at the following scheme in case of constant background f .

Algorithm 0:

Given boundary flux $g = \sum_{j=1}^m g_j$, arising from the m unknown objects each of which is the union of discs) with $f \equiv \text{const}$.

(i) Identify $n = \sum_{j=1}^m n_j \geq m$ equivalent point sources and weights λ_k according to Lemma 2.1 using Algorithm PDAP.

This also yields a decomposition $g = \sum_{k=1}^n g_{pts_k}$ of the given data;

² $L^2(\Sigma)$ regularity of the flux (in spite of the low $W^{1,q}(\Omega)$, $q < \frac{d}{d-1}$ regularity of u) is obtained by bootstrapping from the homogeneous impedance conditions in case of $\Sigma \subseteq \partial\Omega$; otherwise, an assumption of the source domain to be at distance from Σ needs to be imposed in order to be able to invoke interior elliptic regularity.

- (ii) Determine the radii of equivalent discs from weights w_k by resolving the identity (14) for r . rep Y (8)
- Merge these discs into m objects: discs belong to the same object if their intersection is nonempty;
- Assigning discs and therewith equivalent point sources to objects g_{\backslash} for $k \in \{1, \dots, n\} \in \{1, \dots, m\} \in \{1, \dots, p\}$ also yields a decomposition of the given data $g = g = \sum_{\backslash=1}^m g_{\backslash}$, where $g_{\backslash} = \sum_{j=1}^{n_{\backslash}} g_{pts,j}$.
- (iii) For each object D_{\backslash} , $\backslash \in \{1, \dots, m\}$, separately determine the object boundary parametrised by a curve from moment matching (12) data g , using a Newton iteration;

As a starting value for each curve in (iii) we use the disc with the centroid of the union of discs belonging to the \backslash -th object as a center and the radius corresponding to the sum of weights within the \backslash -th object via (14). Alternatively to (iii) one could use algorithms from computational geometry for determining the boundary of a union of discs see, e.g., [14, 16] and the citing literature.

In case of variable background f as relevant here, and/or a set D that is not a finite union of discs the representation by equivalent discs is not exact and therefore the decomposition of the data according to objects is not valid. We therefore replace (iii) by a simultaneous Newton based matching of the flux data g (not of its moments) to the flux data computed from forward simulations according to the collection of parametrised object boundaries. We can still regard the discs obtained by (ii) as good starting guesses for Newton's method and thus proceed as follows.

Algorithm 1:

given boundary flux $g = \sum_{\backslash=1}^P g_{\backslash}$ arising from the m unknown objects D

- (i) Identify $n = \sum_{\backslash=1}^P n_{\backslash} \geq m$ point sources s_k and weights w_k by applying Algorithm PDAP; rep Y (9)
- (ii) Determine disc radii from weights w_k by resolving the identity (14) for r . Merge discs to m objects: discs belong to the same object if their intersection is nonempty;
- (iii) For all objects $D_{\backslash} \in \{1, \dots, m\}$, simultaneously, determine the object boundaries parametrised by curves by matching the combined observational data (6), using a Newton iteration.

The choice of a starting value for (iii) is the same as in Algorithm 0, namely a disc with centre determined as centroid of all discs pertaining to the \backslash -th object and radius determined by using the sum of weights in (14).

2.1 Reconstructions

In this section we show reconstruction of piecewise constant nonlinearity coefficients with supports being inclusions in the unit disk Ω . rep X p.8/9

Our forward solvers for (7), (11) (in the special cases (8), (9) of (7)) rely on the fact that with the fundamental solution to the Helmholtz equation $G(x) = H_0^{(1)}(\tilde{\kappa}|x|)$ in two space dimensions, (with $\tilde{\kappa}$ being the Hankel function of order zero) the solution to rep Y (10)

$$4u^{R^2} + \tilde{\kappa}^2 u^{R^2} = f \quad \text{in } R^2$$

can be determined by convolution $u = G * f$. It thus remains to solve the boundary value problem rep Y (11)

$$4u^d + \tilde{\kappa}^2 u^d = 0 \quad \text{in } \Omega, \quad \partial_\nu u^d + \tilde{\kappa} u^d = g$$

with $g = -\partial_\nu u^{R^2} - \tilde{\kappa} u^{R^2}$, which we do by the integral equation approach described in [12, Sections 3.1, 3.4], that easily extends to the case of impedance boundary conditions. The solution to (7), (11) is then obtained as $u \stackrel{R^2}{=} u^d$. We point to the fact that solving the Helmholtz equation with large wave numbers is a challenging task and a highly active field of research, see e.g. [32, 34, 37] and the references therein. Since our emphasis lies on a proof of concept for parameter identification, we did not implement any of these high frequency solvers here.

In all our reconstructions it is apparent that the point source reconstruction algorithm from [8, 38] combined with the equivalent discs approximation – that is, steps (i) and (ii) in Algorithm 1 – provides an extremely good guess of the curves to be recovered. This is essential for the convergence of Newton's method in view of the high nonlinearity of the shape identification problem.

Using the third harmonic $M = 3$: The reconstructions in Figure 1 are obtained by following the steps of Algorithm 1 at wave number $\tilde{\kappa} = 10$ and then carrying out another Newton step with data from the third harmonic – i.e. at $\tilde{\kappa} = 15$ either (d) sequentially using the result from $m \approx 10$ as a starting value or, (e) applying Newton's method simultaneously to $\tilde{\kappa} = 10$ and $\tilde{\kappa} = 15$. rep Y (14)

The numerical results indicate that the additional information obtained from the next ($m = 3$) harmonic does not yield much improvement. This is due to the lower – by two to three orders of magnitude – intensity of the signal at that higher frequency and seems to confirm the experimental evidence and common practice of skipping higher than second harmonics.

Reconstructions from partial data: In Figures 2, 3 we show reconstructions from partial data, quantified in terms of the relative arc length α of the observation boundary, which is marked in green. The quality appears to decrease only slightly with decreasing amount of data, until at a certain point (between 30 and 40 per cent of full angle, that is, of the whole boundary) the algorithm partially breaks down and fails to find one rep Y (13)
rep Y (12)

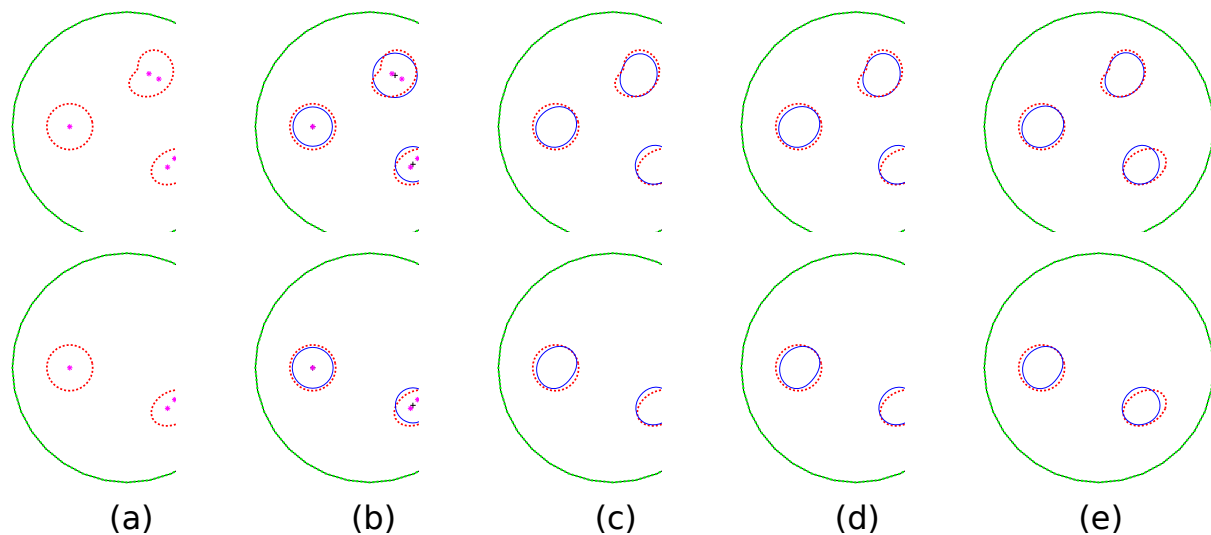


Figure 1: Reconstruction of three (top row) or two (bottom row) inclusions from full data: (a) point sources step (i) of Algorithm 1; (b) equivalent disks step (ii) of Algorithm 1; (c) Newton with second harmonic; (d) Newton with third harmonic; (e) Newton with second and third harmonic.
 green dotted line. . . observation boundary; blue dotted lines. . . actual inclusion boundaries; magenta stars. . . reconstructed point sources; blue solid lines. . . boundary reconstructions

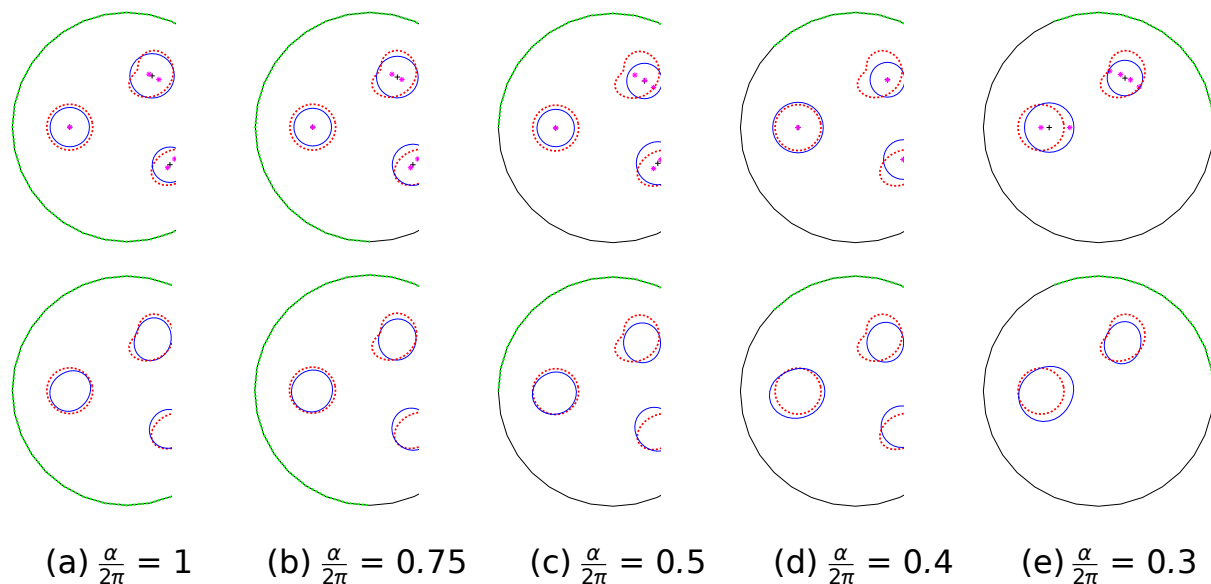


Figure 2: Reconstruction of three inclusions from partial data.
 top row: equivalent point sources and disks;
 bottom row: boundary curves from Newton's method.
 legend: see caption of Figure 1

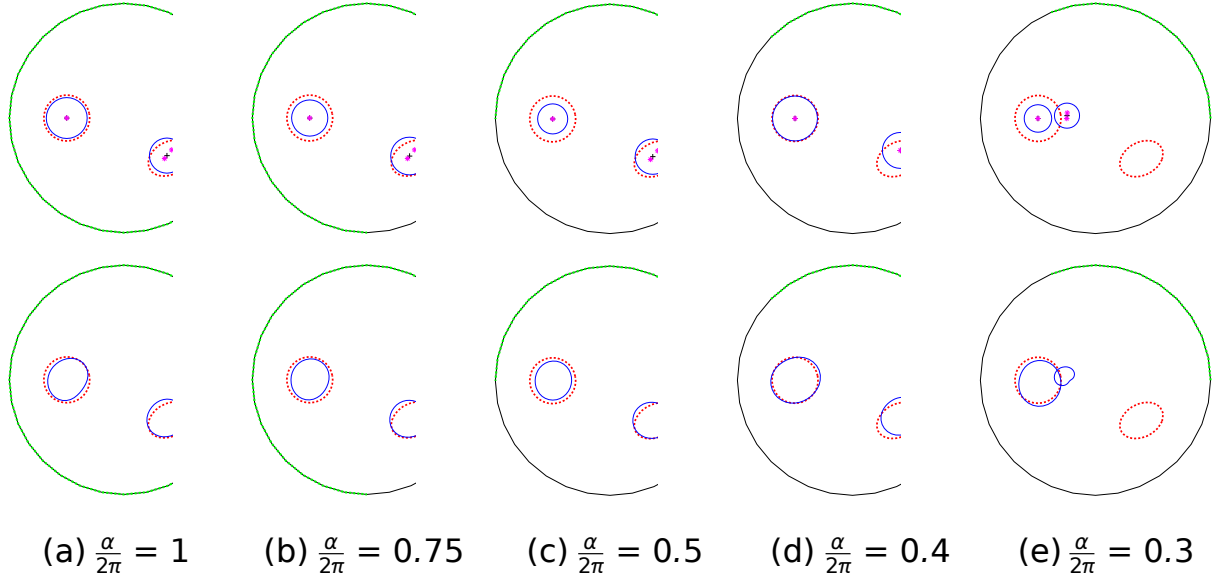


Figure 3: Reconstruction of two inclusions from partial data; top row: equivalent point sources and disks; bottom row: boundary curves from Newton's method; legend: see caption of Figure 1

The ability of an inclusion to stay reconstructible from a low amount of data is related to its weight according to the associated averaging to (13) (using the object's average radius). Figures 2 and 3 these weights are 0.75 for the circle, 0.0692 for the cardioid and 0.0515 for the ellipse. Almost the position relative to the measurement boundary clearly plays a role.

It may seem that simple completion of data from the measurement subarc to the entire boundary should give similar results by for example using the Fourier series expansion. However, this analytic continuation step comes at a price: we have N Fourier modes over an arc of length α then this analytic continuation results from solving a system with a matrix $P(N, \alpha)$ the conditioning of which can be computed analytically. The condition number will increase with both N and decreasing values of $\alpha < 2\pi$. In fact this is a well-understood problem, see [39] where it has been shown that the condition number of $P(N, \alpha)$ is asymptotic (for large N) to

$$c_N \sim e^{\gamma(\alpha)N} \text{ where } \gamma(\alpha) = \log \frac{\sqrt{2 + \sqrt{1 + \cos \alpha}}}{\sqrt{2 - \sqrt{1 + \cos \alpha}}} \quad (15)$$

This has been used in several inverse problems, see, e.g., [20, 33].

However, in our situation the reconstructions are performing much better than the above pessimistic estimate would suggest, due to the fact that our reconstruction does not rely on extending the boundary data but rather on directly applying our method to the restricted flux $g|_{\partial\Omega}$. The additional information that the PDE model provides clearly contributes to this improvement, which is also reflected in the condition number

1 of the Jacobian in Newton's method versus the theoretical prediction for data completion
 from [39] This can be seen in Table 1.

$\frac{\alpha}{2\pi}$	cond(J)	c_N [39]
0.75	29.6	2.8e+2
0.5	64.9	2.3e+5
0.4	73.7	1.8e+07
0.3	1733.8	2.6e+08

Table 1: Condition numbers of Jacobian in Newton's method for a single inclusion using 9 basis functions versus condition number formula (15) for data completion with $N = 9$

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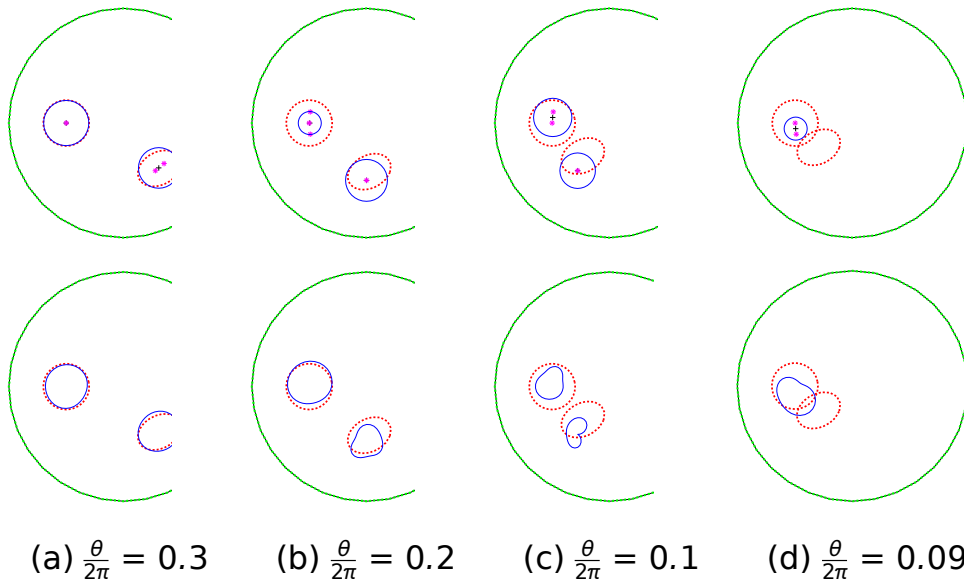


Figure 4: Reconstruction of two inclusions at different distances, top row: point sources and disks, bottom row: boundary curves from Newton's method. legend: see caption of Figure 1

3 **Varying distance between objects** Figure 4 shows reconstructions of two inclusions. 11, 1.1
 4 at several distance, given by the difference θ in the phase of the centroid (in polar coordi-
 5 nates). The given data appears to allow distinction of objects very well as long as they
 6 do not overlap. However, decreasing distance between them compromises the quality of
 7 reconstructions.

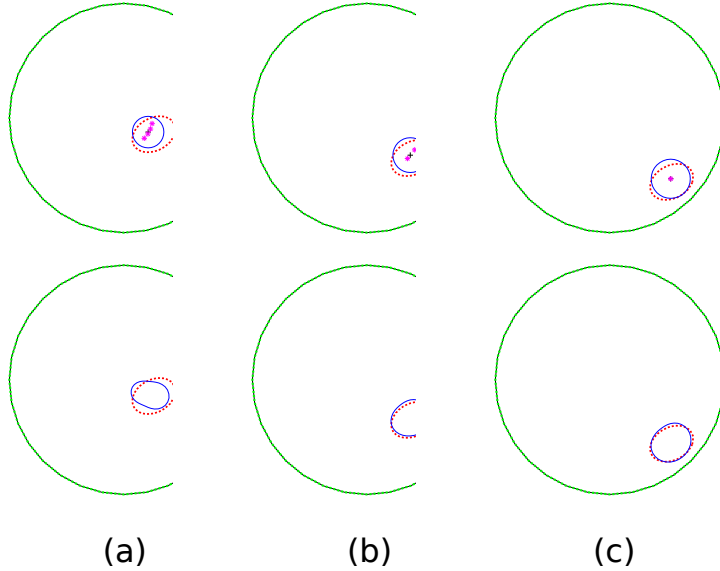


Figure 5: Reconstruction of an inclusion at different distances from the boundary; top row: equivalent point sources and bottom row: boundary curves from Newton's method; legend see caption of Figure 1

Varying distance to boundary

Figure 5 shows reconstructions of an inclusion at several distances from the boundary. The relative error $\frac{kq - q_{\text{act}} k_{L, 2(0, 2\pi)}}{kq_{\text{act}} k_{L, 2(0, 2\pi)}}$ in the boundary parametrisation after application of Newton's method was (a) 0.2963 (b) 0.1931 (c) 0.1434. Also visually, it is obvious that closeness to the observation surface significantly improves the reconstruction quality.

Reconstruction from noisy data

Finally we study the impact of noise in the measurements on the reconstruction quality, see Figure 6 for the case of three objects. Regularisation is mainly achieved by the sparsity prior incorporated via the PDAP point source identification and this actually makes the process very stable with respect to perturbation in the measurements up to noise levels of about three per cent. Using partial data clearly impacts this robustness and thus only works with noise levels of two per cent or less.

3 Convergence of Newton's method

Similarly to the time domain setting [26], one can prove that the all-at-once formulation of this inverse problem (even with arbitrary $M \in \mathbb{N} \cup \{\infty\}$) satisfies a range invariance condition, which, together with a linearised uniqueness result, enables to prove convergence of a regularised frozen Newton method.

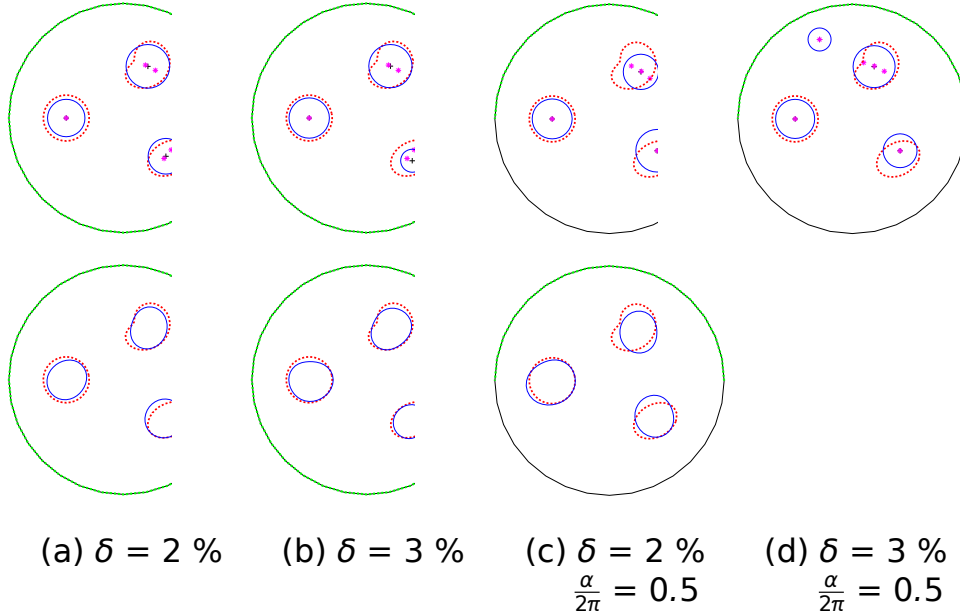


Figure 6: Reconstruction of three inclusions from noisy data. top row: equivalent point sources and disks, bottom row: boundary curves from Newton's method. legend: see caption of Figure 1

We write the inverse problem of reconstructing η in (3) as a nonlinear operator equation

$$\begin{aligned} G_m(\eta, \hat{p}) &= h_m \quad m \in \{1, \dots, M\} \text{ with } \hat{p}_1, \dots, \hat{p}_M \\ C_m \hat{p}_m &= y_m \quad m \in \{1, \dots, M\} \end{aligned} \quad (16)$$

for the model operators $G: Q \times V^M \rightarrow W$ (including the case $M = \infty$ with $(N; V)$ in place of V^M), $h_1 = \hat{h}$, $h_m = 0$ for $m \geq 2$ and the observation operators $C \in \mathcal{L}(V, Y)$. Here Q, V, Y are the parameter, state, and data spaces.

The components G_m of the model part of the forward operator have the particular structure

$$G_m(\eta, \hat{p}) = D_m \hat{p}_m + B_m(\hat{p})\eta \quad (17)$$

with $D_m \in L(V, W)$ and $B(\hat{p}) \in L(Q, W)$ linear for each $\hat{p} \in V^M$ but depending nonlinearly on \hat{p} . (This is different from [25], where we considered a sum of linear operators B in a single model equation rather than a system of model equations.) More concretely, in our setting with the operators defined by

$$\begin{aligned} Au &= \int_{\Omega} \nabla u \cdot \nabla v \, dx + \gamma \int_{\partial\Omega} u v \, ds \\ Du &= \int_{\Omega} \nabla u \cdot \nabla v \, dx + (\beta + b\gamma) \int_{\partial\Omega} u v \, ds, \\ Mu &= \int_{\Omega} u v \, dx + \beta b \int_{\partial\Omega} u v \, ds \end{aligned} \quad (18)$$

1 we take

$$\begin{aligned}
 D_m &= -m^2 \omega^2 M + c^2 A + i m \omega D, \quad C_m = \text{tr}_\Sigma, \\
 B_m(\hat{p})(x) &= m^2 \omega^2 \tilde{B}_m(\hat{p}(x)) \\
 \tilde{B}_m(\sim c) &= \frac{1}{4} \sum_{\ell=1}^{m-1} C_{C_{m-\ell}} + \frac{1}{2} \sum_{k=m+2}^{\infty} 2 \frac{C_{k-m}}{2} C_{\frac{k+m}{2}} \quad M = \infty \text{ (a)} \\
 &\quad \frac{1}{4} \sum_{\ell=1}^{m-1} C_{C_{m-\ell}} \quad M \in \mathbb{N} \cup \{\infty\} \text{ (b)} \quad \sim c \in {}^M C \quad (19) \\
 Q &= L^2(\Omega), \quad V = H^2(\Omega), \quad W = L^2(\Omega), \quad Y = L^2(\Sigma),
 \end{aligned}$$

2 where the first sum over ℓ is empty in the case $m=1$. Here $B_m(\hat{p}) : L^2(\Omega) \rightarrow L^2(\Omega)$ is rep X p.13, (18)
 3 to be understood as a multiplication operator and bounded (i.e. $B_m(\hat{p}) \in \mathcal{B}(L^2(\Omega), L^2(\Omega))$)
 4 follows from the fact that $L^2(\Omega)$ is continuously embedded in $H^2(\Omega)$ and therefore the
 5 functions p as well as their products are in $H^2(\Omega)$. Differentiability of the mappings
 6 follows from their polynomial (in fact, quadratic) structure in our particular setting.

7 We consider both the case (a) that gives full equivalence to the Westervelt equation (16)
 8 and the simplification (b) that corresponds to skipping the under-braced terms in (3) and
 9 is used in our numerical tests. rep X p.13, (18)

10 The abstract structure (16,17) together with an extension of the dependency of
 11 that is, introducing an artificial dependency of η on m to $\tilde{\eta} = (\eta)_{m \in \{1, \dots, M\}} \subseteq Q^M$ allows rep Y (16)
 12 one to more generally establish a differential range invariance relation on a neighbourhood
 13 U of $(\sim p_0)$ rep X p.13, (18)

$$\text{for all } (\sim p) \in U \exists r(\sim p) \in \mathcal{Q} \times V^M : F(\sim p) \hat{=} F(\sigma, \hat{p}) = F^0(\sim p_0) r(\sim p), \quad (20)$$

14 for

$$\begin{aligned}
 F &= (G_m, C_m)_{m \in \{1, \dots, M\}} \quad \hat{p} = (\hat{p}_m)_{m \in \{1, \dots, M\}} \\
 r(\sim p) \hat{=} &(\hat{r}_m(\sim p), \hat{\hat{r}}_m(\sim p))_{m \in \{1, \dots, M\}} \quad (21)
 \end{aligned}$$

15 Indeed, with

$$G_m^0(\sim p_0)(d\eta, \underline{d}) = D_m d\hat{p}_m + \sum_{n=1}^M \frac{\partial B_m}{\partial \hat{p}_n}(\hat{p}_0) d\hat{p}_n \sim \eta_m + B_m(\hat{p}_0) d\eta_m$$

16 and

$$\begin{aligned}
 r_m^{\hat{p}}(\sim p) \hat{=} &\hat{p}_m - \hat{p}_{0,m} \\
 r_m^{\tilde{\eta}}(\sim p) \hat{=} &\eta_m - \eta_{0,m} + B_m(\hat{p}_0)^{-1} (B_m(\hat{p}) - B_m(\hat{p}_0)) \eta_m - \sum_{n=1}^M \frac{\partial B_m}{\partial \hat{p}_n}(\hat{p}_0) (\hat{p}_m - \hat{p}_{0,m}) \eta_{0,m}
 \end{aligned}$$

17 we obtain (20). To this end, we assume that η is chosen such that for each $m \in \{1, \dots, M\}$,
 18 the operator $B_m(\hat{p}_0) : Q \rightarrow W$ is an isomorphism. Under this assumption and if η is
 19 Lipschitz continuously differentiable, the mapping r is close to the shifted identity

1 operator in the sense that

rep Y (17)

$$\begin{aligned}
 & kr(\sim \hat{p}) \hat{=} ((\sim \hat{p}), \hat{=} (\sigma, \hat{p}_0)) k_{Q^M \times V^M} \\
 & = B_m(\hat{p}_0)^{-1} B_m(\hat{p}) - B_m(\hat{p}_0) (\eta_m - \eta_{0,m}) \\
 & \quad + B_m(\hat{p}) - B_m(\hat{p}_0) - \sum_{n=1}^{\infty} \frac{\partial B_m}{\partial \hat{p}_n}(\hat{p}_0) (\hat{p}_m - \hat{p}_{0,m}) \eta_{0,m} \quad m \in \mathbb{N} \setminus Q^M \\
 & \leq C \|\hat{p} - \hat{p}_0\|_{V^M} \|\eta - \eta_0\|_{Q^M} + \|\hat{p} - \hat{p}_0\|_{V^M},
 \end{aligned} \tag{22}$$

2 that is,

$$kr(\sim \hat{p}) \hat{=} ((\sim \hat{p}), \hat{=} (\sigma, \hat{p}_0)) k_{Q^M \times V^M} \leq C \|\sim \hat{p} - (\sigma, \hat{p}_0)\|_{Q^M \times V^M}^2 \tag{23}$$

3 for $C > 0$. Together with $r(\sim \hat{p}_0) = 0$, (23) implies that r is Fréchet differentiable at
 4 $(\sim \hat{p}_0)$ with derivative $r'(\sim \hat{p}_0) = \text{id}_X$, from which one can easily conclude. (cf [28])
 5 that

$$\begin{aligned}
 & \exists \epsilon \in (0, 1) \forall (\hat{p}) \in \hat{U} (\subseteq X) : kr(\sim \hat{p}) \hat{=} r(\sim \hat{p}) - (\sim \hat{p} - \hat{p}_0) k_X \\
 & \leq \epsilon \|\sim \hat{p} - \hat{p}_0\|_X
 \end{aligned} \tag{24}$$

6 in a sufficiently small neighbourhood \hat{U} of $(\sim \hat{p}_0)$

rep X p.14, l.1

7 In our concrete setting (10) where $B_m(\hat{p}_0)$ is the multiplication operator with:
 8 $m^2 \omega^2 \tilde{B}_m(\hat{p}_0(x))$, the isomorphism property means that \hat{p}_0 must be chosen such that for
 9 all $m \in \mathbb{N}$, $0 < \inf_{x \in \Omega} \phi_m(x) \leq \sup_{x \in \Omega} \phi_m(x) < \infty$. This is analogous to the
 10 time domain formulation [28] which is equivalent in case where $\{p_k(t, x)\} =$
 11 $< \sum_{k=1}^{\infty} \phi_k(x) e^{ik\omega t}$ for $p_0(t, x) = < \sum_{k=1}^{\infty} \hat{p}_0 k(x) e^{ik\omega t}$, and where the corresponding
 12 range invariance condition can be proven under the assumption
 13 $0 < \inf_{t \in (0, T)} \inf_{x \in \Omega} \phi_0(t, x) \leq \sup_{t \in (0, T)} \sup_{x \in \Omega} \phi_m(x) < \infty$.

14 Since \tilde{B}_m is polynomial (more precisely quadratic) in its arguments and $\mathcal{V}(\Omega)$ is a
 15 Banach algebra, the operator is Lipschitz continuously differentiable and we have the
 16 following sufficient conditions in terms for (22) (note that the factors ω cancel
 17 out, so we can replace \tilde{B}_m by B_m in (22); moreover, we can exploit symmetry of the first
 18 sum)

$$\begin{aligned}
 & \frac{1}{\tilde{B}_m(\hat{p}_0)} \frac{1}{4} \sum_{n=1}^{\infty} (\hat{p} - \hat{p}_0) \cdot (\hat{p} + \hat{p}_0)_{m-n} \\
 & \quad + \frac{1}{2} \sum_{k=m+2:2}^{\infty} \overline{(\hat{p} - \hat{p}_0)^{\frac{k-m}{2}}} \hat{p}_{\frac{k+m}{2}} + \overline{\hat{p}_0^{\frac{k-m}{2}}} (\hat{p} - \hat{p}_0)^{\frac{k+m}{2}} \quad m \in \mathbb{N} \setminus \{1\} \quad (\mathbb{N}; L^\infty(\Omega)) \\
 & \leq C \|\hat{p} - \hat{p}_0\|_{V^M}
 \end{aligned} \tag{25}$$

19

$$\begin{aligned}
 & \frac{1}{\tilde{B}_m(\hat{p}_0)} \frac{1}{4} \sum_{n=1}^{\infty} (\hat{p} - \hat{p}_0) \cdot (\hat{p} - \hat{p}_0)_{m-n} + \frac{1}{2} \sum_{k=m+2:2}^{\infty} \overline{(\hat{p} - \hat{p}_0)^{\frac{k-m}{2}}} (\hat{p} - \hat{p}_0)^{\frac{k+m}{2}} \quad m \in \mathbb{N} \setminus V^M \\
 & \leq C \|\hat{p} - \hat{p}_0\|_{V^M}^2
 \end{aligned} \tag{26}$$

where the under-braced sum is skipped in case (b).

Since the artificial dependence of $\sim \eta$ on m is clearly unfavourable to uniqueness of this coefficient from the given data, we penalise it by a term $P \sim \eta \in Q$ rep Y (18)

$$(P \sim \eta) = \eta_m - \frac{\sum_{n=1}^M n^{-2} \eta_n}{\sum_{n=1}^M n^{-2}},$$

where the weights n^{-2} in the 2 projection are introduced in order to enforce convergence in case $M = \infty$. Note that the n independent target (η, η, \dots) is clearly not contained in $^2(N; Q)$ but in the weighed space $^2_w(N; Q)$ with weights n^{-2} . We here first of all aim at finding a general $\eta \in Q$. In case we want to reconstruct a piecewise constant coefficient η , we can achieve this by, e.g., adding a total variation term to P .

This penalisation together with condition (20) allows us to rewrite the inverse problem (16) as a combination of an ill-posed linear and a well-posed nonlinear problem

$$\begin{aligned} F^Q(\sim \eta, \hat{p}_0) \hat{r} &= h - F(\sim \eta, \hat{p}_0) \\ r(\sim \eta) &= \hat{r} \\ P \sim \eta &= 0 \end{aligned} \quad (27)$$

for the unknowns $(\sim \eta) \in Q \times Q^M \times V^M$ (or in $^2_w(N; Q) \times ^2_w(N; Q) \times ^2(N; V)$ in case $M = \infty$). Here $(\sim \eta, \hat{p}_0) \in Q \times V^M$ is fixed and in (20) $U \subseteq Q \times V^M$ is a neighbourhood of $(\sim \eta, \hat{p}_0)$.

The following regularised frozen Newton method can then be shown to converge.

$$x_{n+1}^\delta \in \operatorname{argmin}_{x \in U} kF^Q(x_0)(x - \hat{x}_n) + F(\hat{x}_n) - \hat{h}k_Y^2 + \alpha_n k \sim \eta - \hat{\eta}_0 k_Q^2 + kP \sim \eta k \quad (28)$$

where $\hat{h} \approx h$ is the noisy data, $\alpha_n \rightarrow 0$ as $n \rightarrow \infty$, (e.g. $\alpha_n = \alpha_0 n^q$ for some $q \in (0, 1)$), and we abbreviate $x = (\sim \eta, \hat{p}_0)$.

An essential ingredient of the convergence proof is the verification of the fact that the intersection of the nullspaces of $F^Q(x_0)$ and of P is trivial [25, Theorem 2]. For this purpose, we require the following geometric condition on the observation manifold Σ

$$\text{for all } j \in N : \quad \bigwedge_{k \in K} b_k \phi_j^k(x) = 0 \text{ for all } x \in \Sigma \implies b_k = 0 \text{ for all } k \in K \quad (29)$$

in terms of the eigensystem $\{\phi_j^k\}_{j \in N, k \in K}$ of the selfadjoint positive operator A defined by (18). This means that the eigenfunctions should preserve their linear independence when restricted to the observation manifold and trivially holds in 1-d, where $\#K = 1$ for all $j \in N$.

We will assume that the operators A, D, M have the same H -orthonormal eigenfunctions ϕ with the eigenvalues μ of M and ρ of D satisfying

$$\frac{\rho_j}{\lambda_j} = \frac{\rho}{\lambda} \text{ and } \frac{\mu_j}{\lambda_j^2} = \frac{\mu}{\lambda^2} \implies j = \cdot. \quad (30)$$

This is the case, e.g., if $\beta = 0$ in (18), since then with $H = I$ is the identity, $D = bA$ holds, and therefore $\rho = b\lambda$, so that (30) simply becomes $\frac{1}{\lambda_j^2} \Rightarrow j = \cdot$. rep Y (19)

Condition (30) is needed to prove the following linear independence result that will play a role in the linearised uniqueness result Theorem 3.1 which can be found in the appendix.

Lemma 3.1 Let $(\mu_j)_{j \in \mathbb{N}}, (\lambda_j)_{j \in \mathbb{N}}, (\rho_j)_{j \in \mathbb{N}} \subseteq \mathbb{C}$ be sequence of strictly increasing numbers (30) such that (30) holds.

Then

$$\text{for all } m \in \mathbb{N} : 0 = \sum_{j=1}^{\infty} \frac{m^2}{-m^2 \omega^2 \mu_j + c^2 \lambda_j + i m \omega \rho_j} c_j \Rightarrow (c_j = 0 \text{ for all } j \in \mathbb{N})$$

We are now in the position to prove uniqueness for the linearised problem, which, besides being of interest on its own, is also an essential ingredient to the convergence proof of Newton's method.

Theorem 3.1 For (21), (17), (19), with $M = \infty$ and η independent of m (that is, $P \sim \eta = 0$), $\hat{\rho}_0$ chosen such that $\hat{\rho}_{0,m}(x) = \varphi(x) \psi_m$ for some $\varphi \in H^1(\Omega)$, $\varphi \neq 0$ almost everywhere in Ω , $f_m := \tilde{B}_m(\varphi) \in C \setminus \{0\}$ for all $m \in \mathbb{N}$. Then under the linear independence condition (29), with A, D, M simultaneously diagonalisable with (30), the linearisation $(\hat{\rho}_0, \hat{\rho}_0)$ at $\eta = 0$ is injective.

Proof. Using the operators A, D, M as in (18) we can write the condition $(\hat{\rho}_0, \hat{\rho}_0)$ for $\eta = 0$, $\hat{\rho}_{0,m}(x) = \varphi(x) \psi_m$, $f_m = \tilde{B}_m(\varphi)$ as

$$[-m^2 \omega^2 M + c^2 A + i m \omega D] \underline{d\rho}_m + m^2 \omega^2 f_m \varphi \underline{d\eta} = 0 \text{ and } \underline{t}_\Sigma \underline{d\rho}_m = 0 \text{ for all } m \in \mathbb{N} \quad (31)$$

Using the diagonalisation by means of the eigenfunctions ϕ_j^k , $j \in \mathbb{N}, k \in K^j$, by taking the H inner product of (31) with ϕ_j^k , relying on $\underline{d\rho}_m = \sum_{j=1}^{\infty} \sum_{k \in K^j} \underline{h} \underline{d\rho}_m \phi_j^k$ and setting $\underline{a}_j^k = \underline{h} \underline{d\eta} \varphi_j^k \phi_j^k$ we can rewrite this as

$$m^2 \omega^2 f_m \sum_{j=1}^{\infty} \frac{1}{-m^2 \omega^2 \mu_j + c^2 \lambda_j + i m \omega \rho_j} \sum_{k \in K^j} \underline{a}_j^k \phi_j^k(x_0) = 0 \text{ for all } x_0 \in \Sigma, m \in \mathbb{N}.$$

Since the entries $\frac{1}{-m^2 \omega^2 \mu_j + c^2 \lambda_j + i m \omega \rho_j}$ define an infinite generalised Hankel matrix which is therefore nonsingular (see Lemma 3.1), this implies

$$0 = \sum_{k \in K^j} \underline{a}_j^k \phi_j^k(x_0) \quad \text{for all } j \in \mathbb{N}, x_0 \in \Sigma.$$

Using (29), we conclude $\underline{a}_j^k = 0$ for all $j \in \mathbb{N}$, $k \in K^j$ and thus $\underline{d\eta} = 0$. Returning to the first equation in (31) with $\underline{d\eta} = 0$, due to uniqueness of the solution to this linear homogeneous PDE with homogeneous boundary conditions, we also have $\underline{d\rho} = 0$.

According to [25, Theorem 2], we obtain the following

Theorem 3.2 Let $x^\dagger = (\tilde{x}, \tilde{p})$ be a solution to (27) and let for the noise level $\delta \geq k\delta - y_k$ the stopping index $n_*(\delta)$ be chosen such that

$$n_*(\delta) \rightarrow 0, \quad \delta \sum_{j=0}^{n_*(\delta)-1} c^j \alpha_{n_*(\delta)-j-1}^{-1/2} \rightarrow 0 \quad \text{as } \delta \rightarrow 0 \quad (32)$$

with c as in (23). Moreover, let the assumptions of Theorem 3.1 be satisfied with α such that (25), (26) holds for all in a neighbourhood U of

Then there exists $\rho > 0$ sufficiently small that for $x \in B_\rho(x^\dagger) \subseteq U$ the iterates $(x_n^\delta)_{n \in \{1, \dots, n_*(\delta)\}}$ are well-defined by (28), remain in $B_\rho(x^\dagger)$ and converge in $\mathbb{Q} \times V^M$, $kx_{n_*(\delta)}^\delta - x^\dagger k_{Q^M \times V^M} \rightarrow 0$ as $\delta \rightarrow 0$. In the noise free case $\delta = 0$, $n_*(\delta) = \infty$ we have $kx_n - x^\dagger k_{Q^M \times V^M} \rightarrow 0$ as $n \rightarrow \infty$.

Appendix

Proof of Lemma 3.1:

With $w_j(t) := -\mu\omega^2 + \epsilon\lambda_j t^2 + i\omega\rho t$, the premise of the lemma reads as

$$\text{for all } t \in \mathbb{T}_h : m \in \mathbb{N} : 0 = \sum_{j=1}^{\infty} \frac{1}{w_j(t)} c_j.$$

Thus, after multiplication with $\prod_{m \in \mathbb{N}} w_m(t)$ and with $W(t) := \prod_{j=1}^{\infty} w_j(t)$ we get

$$\text{for all } t \in \mathbb{T}_h : m \in \mathbb{N} : 0 = W(t).$$

Since W is analytic, this implies that $W \equiv 0$ on all of \mathbb{C} . Choosing $t_k = -\frac{i\omega}{2\epsilon} \frac{\rho_k \mp \sqrt{\rho_k^2 - \mu_k}}{\lambda_k}$ as the roots of w_k we obtain

$$\text{for all } k \in \mathbb{N} : \sum_{m=k}^{\infty} w_m(t_{k\pm}) c_m = 0 \quad (33)$$

A small side calculation yields that under condition (30), the roots of the functions w are distinct for different j :

$$\begin{aligned} t_{j+} = t_+ \text{ and } t_{j-} = t_- &\Rightarrow t_{j+} + t_{j-} = t_+ + t_- \text{ and } t_{j+} - t_{j-} = t_+ - t_- \\ &\Rightarrow \frac{\rho_j}{\lambda_j} = \frac{\rho}{\lambda} \text{ and } \frac{\mu_j}{\lambda_j^2} = \frac{\mu}{\lambda^2}, \end{aligned}$$

which by (30) implies $j = \cdot$.

Hence, $w_m(t_{k\pm}) \neq 0$ and from (33) we conclude that for all $k \in \mathbb{N}$.

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