Department of Mathematics and Systems Analysis

Inverse Source Methods in Diffuse Imaging

Lauri Harhanen

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Lauri Harhanen

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Abstract

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Abstract

This dissertation studies methods for inverse source problems in diffuse imaging. The convex source support method for the Poisson's equation is extended to the two-dimensional half-space and a ball in three dimensions. The related problems of detecting inhomogeneities in electrical impedance tomography are discussed, as well. In addition to using the conventional measurements consisting of one or more Cauchy data pairs, sweep data, a novel measurement configuration compatible with the convex source support algorithm, is proposed and analyzed.

This treatise also considers an amalgamation of non-linear Tikhonov regularization and preconditioned Krylov subspace methods. The lagged diffusivity fixed point iteration is used to produce a sequence of least-squares problems with linearized regularizers. These regularizers are recast as preconditioners. A modified version of the LSQR algorithm is derived, allowing efficient use of the introduced preconditioners. While the performance of the resulting algorithm is tested on fluorescence diffuse optical tomography, the method is directly applicable to other linear inverse problems, as well.

Keywords inverse source problems, electrical impedance tomography, convex source support, LSQR, preconditioning

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Tekijä
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Väitöskirjan nimi
Käänteislähdemenetelmiä diffusiiviseen kuvantamiseen

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Tiivistelmä

Tämä väitöskirja käsittelee diffusiivisen kuvantamisen käänteislähdeongelmille tarkoitettuja menetelmiä. Poissonin yhtälölle muokattu konveksin lähteenkantajan menetelmä laajennetaan puolitason ja kolmiulotteisen pallon tapauksiin. Näihin läheisesti liittyviä impedanssitomografian ongelmia lähestytään kahdella tavalla. Tavanomaisten Cauchyn reuna-arvoparimittausten lisäksi tutkitaan uutta pyyhkäisymittaustekniikkaa, ja kumpaankin mittaustapaan sovelletaan konveksin lähteenkantajan menetelmää.

Lisäksi esitetään Tikhonov-regularisoinnin ja pohjustettujen Krylov-aliavaruusalgoritmien yhdistämiseen perustuva menetelmä. Menetelmä käyttää viivästetyn diffusiivisuuden kiintopisteiteraatiota regularisaatiotermin linearisointiin. Syntyvien tehtävien regularisoijia käytetään pohjustimina, ja pohjustettujen tehtävien tehokasta ratkaisua varten johdetaan LSQR-algoritmista uusi, tähän tarkoitukseen hyvin soveltuva muoto. Vaikka johdetun menetelmän tehokkuutta esitellään optisen fluoresenssitomografian avulla, on se suoraan sovellettavissa muihinkin lineaarisiin käänteisongelmiin.

Avainsanat käänteislähdeongelmat, impedanssitomografia, konveksi lähteenkantaja, LSQR, pohjustus

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Preface

This dissertation was written during the years 2008–2013 at the Department of Mathematics and Systems Analysis, Aalto University. I acknowledge the financial support for my work from Finnish Doctoral Programme in Computational Sciences (FICS), Finnish Doctoral Program in Inverse Problems, the Finnish Cultural Foundation and the Magnus Ehrnrooth foundation.

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Finally, I express my gratitude to my family for all the encouragement and support they have given me.

Espoo, November 7, 2013,

Lauri Harhanen

Contents

List of Publications

This thesis consists of an overview and of the following publications which are referred to in the text by their Roman numerals.

I Lauri Harhanen and Nuutti Hyvönen. Convex source support in half-plane. *Inverse Problems and Imaging*, 4(3), 429–448, 2010.

II Harri Hakula, Lauri Harhanen and Nuutti Hyvönen. Sweep data of electrical impedance tomography. *Inverse Problems*, 27(11), 115006 (19pp), 2011.

III Martin Hanke, Lauri Harhanen, Nuutti Hyvönen and Eva Schweickert. Convex source support in three dimensions. *BIT Numerical Mathematics*, 52(1), 45–63, 2012.

IV Simon R. Arridge, Marta M. Betcke and Lauri Harhanen. A priorconditioned LSQR algorithm for linear ill-posed problems with edge-preserving regularization. *arXiv:1308.6634*, 22pp, 2013.

Author's Contribution

Publication I: "Convex source support in half-plane"

The author is responsible for a major part of the analysis, and all of the numerical computations are due to the author.

Publication II: "Sweep data of electrical impedance tomography"

The author's contribution consists of a part of the analysis and all of the numerical computations, the (forward) complete electrode simulations notwithstanding.

Publication III: "Convex source support in three dimensions"

A major part of the analysis and all of the numerical results are due to the author.

Publication IV: "A priorconditioned LSQR algorithm for linear ill-posed problems with edge-preserving regularization"

The author is responsible for a large portion of the presented results.

1. Introduction

Imaging methods are not only an integral part of modern medicine, but also broadly used by the industry in, e.g., non-destructive testing, process tomography, and geological exploration. The renowned computerized tomography (CT), magnetic resonance imaging (MRI), and ultrasonography are accompanied by positron emission tomography (PET), impedance and capacitance tomography, elastography, optoacoustic imaging, optical tomography, and several others. Many of these modalities have both medical and industrial applications and, from the mathematical point of view, they are inverse problems: The aim is to deduce some physical quantity from indirect measurements. For example, CT scanners reconstruct the mass absorption coefficient inside a patient from x-ray projection images.

Inverse problems can also be described as the complements of direct problems. Although this dichotomy is not always obvious, the problem considered direct is often the one where the aim is to solve the result of a law of the nature. These laws are usually expressed as partial differential equations, which are both local and causal. Consequently, they usually possess favorable stability and uniqueness properties. In contrast, inverse problems most often lack several of the desirable features of direct problems, and hence are significantly more involved to solve.

This thesis focuses on three problems in diffuse imaging where the measured physical phenomena is either light or electrical potential. These problems are characterized by the extreme spreading, or diffusion, occurring in the modeled field. The proposed methods are devised for inverse source problems: The measured fields are not directly created by an external device like an x-ray tube in CT, but they are caused by phenomena that are (at least to some extent) endogenous to the subject. For example, neural activity in the brain acts as a source in electroencephalography (EEG), creating electrical potentials which are measured on the scalp. These measurements are then processed to give information on the brain activity.

First, we consider a problem that is related to EEG: the inverse source problem for the Poisson's equation in the framework of electrostatics. We provide two extensions to an algorithm for obtaining certain information, called the convex source support, on the location of an unknown source. Second, we employ reformulations of two specific cases of electrical impedance tomography (EIT) where an inclusion in an otherwise homogeneous domain is re-interpreted as an electrostatic source. The convex source support method is tested on both of the resulting inverse source problems. Finally, we propose a numerical method for fluorescence diffuse optical tomography (FDOT), where the light propagation is modeled using the (stationary) diffusion equation. The proposed method is directly applicable to other linear inverse problems, as well.

2. Convex source support method for the Poisson's equation

The article [23] studied the inverse source problem for the Poisson's equation

$$\Delta u = F \quad \text{in } D, \qquad \frac{\partial u}{\partial \nu} = 0 \quad \text{on } \partial D, \qquad \int_{\partial D} u \, \mathrm{d}s = 0 \tag{2.1}$$

in a two-dimensional, bounded, convex domain D. Since the distributional, compactly supported, mean-free source term F is not uniquely determined by the boundary potential $u_{|\partial D}$, it is essential to consider what can be deduced about F given $u_{|\partial D}$.

A similar situation is faced also in the framework of inverse source and scattering problems for the Helmholtz equation

$$(\Delta + k^2)u = F, \tag{2.2}$$

coupled with the Sommerfeld radiation condition. Under certain assumptions, the amplitude u of a time-harmonic wave satisfies (2.2), where k denotes the wave number and the main interest is the source F [13]. In addition to being an actual source, F can also represent a secondary source that is induced as an incoming wave interacts with a scatterer. These inverse problems for the Helmholtz equation are often studied in an unbounded domain, and the data are assumed to be so called far field patterns, or the asymptotic behavior of the outgoing part of u. This corresponds to measurements made far away from the scatterer. The articles [19, 33, 34, 43, 49] developed the concept of convex scattering support and a method for its estimation from the corresponding far field pattern. Described briefly, the convex scattering support is the smallest convex set which (almost) supports a source compatible with the data.

In [23], the convex scattering support was adapted for the Poisson's equation (2.1). Let us denote the related virtual measurement operator by L, that is, $LF := u_{|\partial D}$ with u solving (2.1) for the source $F \in \mathscr{E}'_\diamond(D)$, where $\mathscr{E}'_\diamond(D)$ denotes the space of compactly supported, mean-free distributions. Using L, [23] defined the convex source support of a boundary potential $g \in \mathscr{R}(L)$ as

$$\mathscr{C} g := \bigcap_{LF=g} \operatorname{supp}_c F, \tag{2.3}$$

where $\mathrm{supp}_c F$ denotes the convex hull of the support of F. Note that the intersection is taken over all the sources that result in the boundary data g. The convex source support has several interesting properties [23]: In brief, for any $g \in \mathscr{R}(L)$ and any $\epsilon > 0$, there exists $F_\epsilon \in \mathscr{E}'_\diamond(D)$ such that $LF_\epsilon = g$ and

$$\mathscr{C}g \subset \mathrm{supp}_c F_\epsilon \subset N_\epsilon(\mathscr{C}g),$$

where $N_\epsilon(\mathscr{C}g)$ denotes the open ϵ-neighborhood of $\mathscr{C}g$. Moreover, $\mathscr{C}g = \emptyset$ if and only if $g \equiv 0$. This means that for any non-trivial boundary potential measurement g, there exists a non-empty unique minimal convex set $\mathscr{C}g$ whose any ϵ-neighborhood supports a source compatible with the observed potential.

2.1 Approximating the convex source support

The methods for computing approximations of the convex scattering and source supports for the two-dimensional setting, presented in [33, 34] and [23], rely on investigating the Fourier coefficients of the measurements. Let us denote the virtual measurement operator for the Helmholtz equation (2.2) by L_k, that is, the far field α of the solution u to (2.2) for F is given by $\alpha = L_k F$. In [34], a Picard test was given for determining if B_R, the origin-centered disc of radius R, contains the convex scattering support of a given far field pattern. To be precise, there exists a source $F_R \in H_0^s(B_R)$ such that $\alpha = L_k F_R$ if and only if

$$\sum_{j=-\infty}^{\infty} \frac{|\alpha_j|^2}{|j|^{-2s} \int_0^R |J_j(kr)|^2 r \mathrm{d}r} < \infty, \tag{2.4}$$

where α_j are the Fourier coefficients of α and J_j represents the Bessel function of the first kind and of order j.

A very similar test is derived in [23] for the convex source support in the case where the domain D is the unit disc: With $\overline{B}_R \subset D$ and denoting the Fourier coefficients of g by g_j, $\mathscr{C}g \subset \overline{B}_R$ if and only if

$$\sum_{j=-\infty}^{\infty} \frac{|g_j|^2}{(R+\epsilon)^{2|j|}} < \infty \tag{2.5}$$

for every $\epsilon > 0$. Although the tests given in [33, 34] and [23] are derived using dissimilar techniques, the resulting tests differ only by the scalings applied to the Fourier coefficients.

Since any practical test can employ only a finite number of Fourier coefficients, the conditions (2.4) and (2.5) must be approximated. In [34], a simple thresholding test was introduced as a method for estimating the smallest R for which (2.4) converges. In contrast, [23] employed a geometrically decreasing model $\log|g_j| \approx m|j| + b$ for the behavior of the Fourier coefficients as suggested in [4]. This reduces the summation in (2.5) into a geometric series, from which we obtain the smallest possible radius $R = e^m$.

The above procedures are valid for testing origin centered discs. Naturally, the methods are viable for detecting sources only if more detailed information can be extracted. For the Helmholtz equation, this is straightforward: The far field pattern is actually the restriction of the Fourier transform of F to the circle of radius k, i.e., $\alpha(\theta) = \mathscr{F}F(k\theta)$, where θ is the polar angle. Hence, the effect of the translation $x \mapsto x + c$ on the far field pattern can be computed by multiplying α with the function $\exp\big(ik|c|\cos(\theta - c/|c|)\big)$.

In the case of the Poisson's equation, a standard tool from (two-dimensional) potential theory allows the extraction of further information on the convex source support of g: By using a suitable Möbius transformation $\Phi : D \to D$ from the unit disc onto itself, the original problem (2.1) can be mapped into a new problem with the transformed source term $(|\det \Phi'|^{-1} F) \circ \Phi^{-1}$ and boundary data $g \circ \Phi^{-1}$. By applying the test (2.5) to the transformed data, one obtains a origin-centered, closed disc B containing $\mathscr{C}(g \circ \Phi^{-1})$, and, consequently, $\Phi^{-1}(B)$ contains $\mathscr{C}g$. This procedure allows one to test if $\mathscr{C}g$ is a subset of any given closed disc $B \subset D$, leading naturally to the concept of discoidal source support, which is the intersection of all discs $B \subset D$ that contain $\mathscr{C}g$. In practice, one is only able to use a finite number of Möbius transformations, and hence only compute an estimate of the discoidal source support.

Domains more complex than a disc can be treated by solving a well-posed transmission problem in order to obtain a virtual boundary potential on the boundary of a large enough disc [24]. In principle, this technique also allows one to obtain more detailed reconstructions of $\mathscr{C}g$ since the extended domain can be arbitrarily large and thus contain larger test discs. However, numerical reasons impose a limit on the maximum size of usable extended domains [24].

2.2 Extension to an unbounded domain

Publication I considered the inverse source problem for the Poisson's equation in an unbounded domain $D \subset \mathbb{R}^2$. More precisely, the domain is assumed to be the upper half-plane, and the third condition of (2.1) is replaced with

$$\lim_{|x| \to \infty} |u(x)| = 0.$$

Although [23] assumed boundedness, most of the results actually hold also for unbounded domains.

Even though it may seem like the simplest approach, using a single Möbius transformation Φ to map the half-plane onto the unit disc and then use the methods from [23] does not result in a desirable algorithm. This is due to the fact that the preimage of $\operatorname{supp}_c(|\det \Phi'|^{-1}F)\circ\Phi^{-1}$ may be non-convex. Hence, such an algorithm would not approximate the discoidal nor convex source support of the boundary measurement, although it would carry some information on the source. Consequently, Publication I employed a family of Möbius transformations to build a technique for approximating the discoidal source support. The resulting algorithm is able to produce useful reconstructions using observations only from one side of the examined domain.

2.3 Extension to a three-dimensional domain

Although [23] considered only two-dimensional domains, the main theoretical results hold also for three spatial dimensions. However, the presented reconstruction algorithm is inherently two-dimensional due to the utilization of Möbius transformations. Publication III extended the algorithm to three dimensions by replacing the Picard test for Fourier coefficients with a test employing spherical harmonics coefficients and using Kelvin transforms

$$\left(\mathscr{K}_{m,b}u\right)(x) := \frac{b}{|x-m|}u(\mathscr{I}_{m,b}(x))$$

instead of Möbius transformations. Note that even though $\mathscr{I}_{m,b}$, the inversion by a sphere with center m and radius b, is a conformal mapping in $\mathbb{R}^3$, the composition $u\circ\mathscr{I}_{m,b}$ is not harmonic for a harmonic u, whereas $\mathscr{K}_{m,b}u$ is. By choosing suitable spheres, one can construct a family of inversions that map the unit ball onto itself and use the associated Kelvin transforms to deal with non-concentric test balls. However, there is a notable difference compared to the two-dimensional case: Kelvin transforms do not retain the homogeneous Neumann boundary condition of (2.1), which must be accounted for in the convergence tests.

3. Convex source support method for electrical impedance tomography

The Calderón problem [5], or EIT, refers to the task of determining the bounded conductivity field σ (with a positive lower bound) from the boundary measurements $v^f_{|\partial D}$ of the functions v^f satisfying the conductivity equation

$$\nabla \cdot \sigma \nabla v = 0 \quad \text{in } D, \qquad \sigma \frac{\partial v}{\partial \nu} = f \quad \text{on } \partial D \tag{3.1}$$

for some mean-free boundary currents f. The problem has received broad interest, and results, both theoretical and practical, have been published in numerous research articles [3, 11, 50]. Our contribution to the Calderón problem consists of two different techniques for applying the convex source support method in EIT.

3.1 Reformulation as an inverse source problem

First, we choose a feasible boundary current f and denote by v_0 the associated background solution, that is, the function satisfying (3.1) for $\sigma \equiv 1$. Assuming that the actual aim is to locate an inclusion in an otherwise homogeneous medium with unit conductivity, we face a problem where $\sigma = 1+\sigma_i$ and the inhomogeneity σ_i is compactly supported in D. By denoting the difference potential with $w := v - v_0$, one obtains

$$\Delta w = -\nabla \cdot \sigma_i \nabla v \quad \text{in } D,$$

where v is the solution to (3.1) for $\sigma = 1+\sigma_i$. The virtual source $F_v = -\nabla \cdot \sigma_i \nabla v$ is clearly supported within the support of σ_i. Hence, methods that are used for localizing sources can also be utilized for approximating the support of σ_i.

The combination of this approach with the convex source support was first published in [24], which assumed that D is a two-dimensional, bounded domain. Publications I and III employed the (reformulated) method in a half-plane and a three-dimensional ball, respectively, using a single boundary current pattern injected with just two electrodes. (It can be thought that a third electrode is moved along the boundary to measure the potential.)

Because different boundary currents result in different potentials v, it is possible to obtain further information on the support of σ_i by using several boundary currents. For each f, one obtains a subset of $\operatorname{supp}_c \sigma_i$. Therefore, by taking the union of all such subsets, a larger and thus more accurate approximation is obtained, cf. [43] for an analogous result in the framework of the Helmholtz equation.

3.2 Sweep data

Publication II introduced an alternative measurement configuration for EIT in two dimensions. Instead of using a single current pattern and measuring the corresponding potential on the whole boundary, we use one fixed and one moving electrode, apply a unit current between the two electrodes, and measure the resulting (relative) potential difference. This measurement, considered as a function of the moving electrode, is called the sweep data. Assuming point-like electrodes (cf. [22]), the sweep data can be given in the form

$$\varsigma(y) = (v^y - v_0^y)(y) - (v^y - v_0^y)(y_0), \qquad y \in \partial D.$$

The potentials v^y and v_0^y satisfy (3.1) for $\sigma = 1 + \sigma_i$ and $\sigma = 1$, respectively, with the current pattern $f = \delta_y - \delta_{y_0}$. Here, the point-like electrodes are modeled as Dirac delta distributions on ∂D with the singularity lying at the position indicated by the subscript. Obviously, in order to employ such data, one must have access to the reference data with a homogeneous conductivity either through time difference imaging or simulations.

In Publication II, we were able to show that the sweep data can, in essence, be continued as a holomorphic function to the complement of $\operatorname{supp} \sigma_i$. Because the continuation is unique and its real part is harmonic, the convex source support algorithm can be applied to the sweep data to obtain an estimate for the location of the inclusion. Since the proof of the harmonic continuation relies strongly on complex analysis, it is currently not known if the results can be extended to three spatial dimensions.

Closely related results for the so-called backscatter data of EIT are available in [25, 26, 27, 30]. The backscatter data can be approximated in practice by rotating a small probe of two electrodes around D and measuring the voltage required for maintaining fixed current between them.

4. Priorconditioned Krylov subspace methods for fluorescence diffuse optical tomography

4.1 Fluorescence diffuse optical tomography

The goal of optical tomography is to determine the optical properties of an object by illuminating it with light and measuring the resulting photon density at the surface. In many applications, the considered media are turbid and, consequently, the propagation of light can be accurately modeled with the diffusion approximation for the radiative transfer equation. For a diffusion coefficient σ and an absorption coefficient μ, the photon density u satisfies

$$\begin{aligned} \left(-\nabla\cdot\sigma\nabla+\mu\right)u &= q \quad \text{in } D,\\ u+2\zeta\sigma\frac{\partial}{\partial\nu}u &= g \quad \text{on } \partial D, \end{aligned} \tag{4.1}$$

where ζ describes the reflectiveness of the boundary. Illumination can either be modeled as an inhomogeneous source term $q \neq 0$ or a suitable boundary value $g \neq 0$. Further details can be found in the extensive review article [1] and the references therein.

Advances in the design of optical marker substances have drawn attention to optical molecular imaging, which allows the study of certain functional processes and pathologies in living subjects. Its main advantages in comparison to many other imaging modalities are the non-invasiveness and high sensitivity that can be achieved at low cost. In contrast, the widely used PET and CT scanners are expensive and expose the patient to harmful, ionizing radiation. While several other phenomena can provide contrast [55], we concentrate on fluorescence diffuse optical tomography (FDOT), where the fundamental idea is to inject the subject with a fluorescent marker substance that targets the interesting molecules. When the subject is subsequently illuminated with excitation light field at a wave length λ_e, the fluorophore, or marker, absorbs light and re-emits photons at a different wave length λ_f. This effectively creates sources inside the subject. Since the two fields are at different wave lengths, it is possible to separate the two photon densities with filters. Important applications for FDOT include small animal imaging [31, 36, 37, 38, 56] and breast tumor detection [14, 39, 51].

Often, the fluorophore concentration is small enough to have a negligible effect on the diffusion and absorption coefficients, and hence the photon density field u_f arising from fluorescence satisfies (4.1) for $q = hu_e$ and $g \equiv 0$, where u_e is the excitation photon density field and h is the main object of interest, the fluorescence yield coefficient. If one knows a priori the diffusion and absorption coefficients — such knowledge could be obtained using optical tomography or some other modality — the problem of FDOT is reduced into the following diffuse, linear inverse source problem: Find the fluorescence yield coefficient h that results in the measurements MGh, where M is the measurement operator (see Publication IV) and G maps h to the induced photon density field u_f solving (4.1). This subproblem was the initial target for the results in Publication IV. However, it became obvious that the same techniques could be used for other inverse problems as well, shifting the presentation of Publication IV into a more general direction.

Although the fluorescence yield coefficient is in many applications compactly supported and localized in the same sense as sources and conductivity inhomogeneities in Chapters 2 and 3, it is not currently known if the convex source support method can be extended to cover FDOT. As noted in [33], the convex scattering support is a flexible theoretical concept, allowing extensions to several problems. However, it is unclear how to devise an efficient algorithm for computing the convex source support in FDOT. This is because of the absorption, which, some very exceptional cases notwithstanding, differs from zero everywhere and hence destroys the harmonicity of the photon density field. Consequently, the reconstruction algorithms relying on Möbius transformations and Kelvin transforms cannot be applied to FDOT. For this reason, we approach FDOT from an alternative perspective. By adding regularization, the original ill-posed problem is replaced with a well-posed one that is (in some sense) closely related to the original. A treatise on such regularization methods, including the two discussed in this section, can be found in [17].

4.2 Tikhonov regularization and truncated Krylov methods

Assuming that the matrix A is a discretization of the compound forward-measurement operator MG, the problem of FDOT is reduced into solving a system of ill-posed linear equations

$$Ax = y, \tag{4.2}$$

where x and y represent the (discretized) fluorescence yield coefficient and the available noisy measurements, respectively. Because the measurement and discretization errors may push y outside the range of A, it is natural to consider the associated normal equations

$$A^{\mathrm{T}}Ax = A^{\mathrm{T}}y. \tag{4.3}$$

Unfortunately, these equations are even more ill-posed than (4.2) due to the squaring of A which squares also the condition number of the problem. A common technique for regaining well-posedness is to use Tikhonov regularization, that is, to add a penalty term and then seek the minimizer of

$$\|y - Ax\|^2 + \alpha R(x), \quad \alpha > 0. \tag{4.4}$$

While it is common to use quadratic penalty terms, i.e., $R(x) = x^{\mathrm{T}}Hx$ or $R(x) = \|Lx\|^2$ because they reduce the minimization of equation (4.4) to a linear problem, such penalties are somewhat restricted. In fact, many often used penalty terms such as Perona–Malik anisotropic diffusion [42] and total variation [44] are non-quadratic. However, the minimization problems corresponding to such penalties are non-linear and hence significantly harder to solve.

An alternative option is to solve (4.3) using a Krylov subspace method such as conjugate gradient (CG) [29] and to regularize through early truncation [21]. This approach is equivalent to minimizing $\|y-Ax\|$ in a low dimensional Krylov subspace

$$\mathscr{K}_m = \mathrm{span}\{A^{\mathrm{T}}y, A^{\mathrm{T}}AA^{\mathrm{T}}y, \ldots, (A^{\mathrm{T}}A)^{m-1}A^{\mathrm{T}}y\}.$$

For comprehensive monographs on the subject, see [46, 52]. Preconditioning is essential in the successful use of Krylov subspace methods in large scale problems [2]. Because fast convergence is guaranteed only if the eigenvalues of the coefficient matrix are clustered (away from zero), preconditioners aim to make the spectrum narrower by substituting

$$P^{-1}A^{\mathrm{T}}Ax = P^{-1}A^{\mathrm{T}}y$$

for (4.3). For well-posed problems this goal is most commonly achieved by taking the preconditioner P to be an inexpensively invertible, crude approximation of the coefficient matrix $A^{\mathrm{T}}A$.

For ill-posed problems, convergence and preconditioning are especially intricate. While the rapid decay of eigenvalues indicates a desperate need for preconditioning, it is not practical to try to cluster the eigenvalues since it would cause overwhelmingly high amplification of noise. The main objective in Publication IV was to derive a technique that combines Tikhonov regularization with Krylov subspace methods in a computationally efficient manner.

4.3 Priorconditioned LSQR

Normal equations (4.3) are encountered so often that a specialized variant of CG has been derived for them. Although normal equations can be solved using the standard CG, the squaring of the coefficient matrix makes them considerably more ill-posed than the original equation (4.2). Instead of applying the Lanczos algorithm [35] to $A^{\mathrm{T}}A$ as in CG, analytically equivalent but numerically more stable method is obtained by using the Golub–Kahan bidiagonalization [18] on A. This modified CG algorithm is called LSQR [40, 41], and is used in Publication IV for solving the fluorescence yield coefficient. Similar to CG, LSQR performs best when accompanied with a good preconditioner. Since traditional preconditioning is not applicable to inverse problems, an alternative stance is taken here.

In [6, 7, 8, 9, 10], inverse problems were considered using the Bayesian paradigm and smoothness priors. On structured grids, an unnormalized smoothness prior p is typically defined through the negative logarithm of its probability density function

$$-\log p(x) \propto \|Dx\|^2, \tag{4.5}$$

where D represents a discretized differential operator. On unstructured grids, differential operators naturally occur in a form leading to priors given as

$$-\log p(x) \propto x^{\mathrm{T}}Hx. \tag{4.6}$$

These priors coincide with a family of extensively used quadratic Tikhonov smoothness penalty terms, cf. Section 4.2. Their motivation arises from the fact that naive, unregularized solutions to ill-posed problems are typically extremely oscillating, which usually contradicts with the reality. The strong oscillations can be removed by imposing (some degree of) smoothness on the solution.

The definitions (4.5) and (4.6) lead to zero-mean Gaussian priors with the unscaled covariances $(D^{\mathrm{T}}D)^{-1}$ and H^{-1}, respectively. The corresponding maximum a posteriori estimate is computed by solving

$$(A^{\mathrm{T}}A + \alpha H)x = A^{\mathrm{T}}y, \tag{4.7}$$

where we have assumed $H = D^{\mathrm{T}}D$. Note that (4.7) is equivalent to the least-squares problem

$$\begin{pmatrix} A \\ \sqrt{\alpha}D \end{pmatrix} x = \begin{pmatrix} y \\ 0 \end{pmatrix}.$$

Motivated by the fact that solving (4.7) for large scale inverse problems requires iterative methods and preconditioning, [6, 7, 8, 9, 10] introduced priorconditioning: They demonstrated that the inverse of the covariance matrix is a powerful preconditioner for solving (4.7) with CG. These results have a strong connection to [8, 20, 28], where differential operators were studied as preconditioners for ill-posed problems from another perspective.

However, there are some issues with the efficient implementation of the aforementioned priorconditioning schemes on unstructured grids. The least-squares connection indicates that LSQR would be better suited for solving (4.7) than CG, but the standard LSQR algorithm [40, 41] assumes that the preconditioning is implemented symmetrically, i.e., by effectively substituting AP^{-1} for A. On structured meshes, this is achieved by setting $P = D$, and it is possible to employ a weighted pseudoinverse if D is non-invertible [16, 32]. On unstructured grids, symmetric preconditioning of LSQR requires the Cholesky (or some other suitable symmetric) decomposition of H. Especially for problems in three spatial dimensions, such a decomposition is prohibitively expensive to compute. To remedy this issue, Publication IV derived a version of LSQR which uses an H-weighted inner product instead of the standard one, which allows us to use H as a preconditioner without its Cholesky decomposition. The factorization-free priorconditioning of LSQR provides a significant advantage: H is often (smoothness priors, Perona–Malik, total variation, etc.) a discrete partial differential operator, which can be inverted by efficient solvers designed specifically for partial differential equations.

Special care must be taken when methods such as multigrid are employed to compute the effect of multiplying a vector by the inverse of the preconditioner P. Indeed, CG and LSQR work only with symmetric, constant preconditioners, but most iterative solvers approximate inverses with matrices that actually depend also on the vector to which the inverse is applied and not only on the matrix that is being inverted. Moreover, the approximate inverse may be non-symmetric even for symmetric matrices. While there exist flexible variants of Krylov subspace methods that allow non-constant preconditioners [45, 47], they arguably provide no advantages over the approach taken in Publication IV: A simple, computationally low-cost single V-cycle multigrid scheme was sufficient for achieving effective priorconditioning.

4.4 Lagged diffusion iteration and priorconditioning

For a quadratic penalty R, the minimizer of (4.4) is simple to find by solving a linear problem giving the critical point of (4.4). For a non-quadratic R, minimization is a non-linear problem and must be solved iteratively. By setting the gradient of (4.4) to zero, one obtains

$$A^{\mathrm{T}}Ax + \alpha\nabla R(x) = A^{\mathrm{T}}y.$$

In many cases, including total variation and Perona–Malik regularization, the gradient of R corresponds to operating on x with an inhomogeneous diffusion operator whose diffusion coefficient depends on x. The minimizer can be computed, for example, using the lagged diffusivity fixed point iteration [53, 54]. An equivalent method can also be derived as a Gauss–Newton type algorithm by using a sparse approximation for the Hessian of R [15]. The resulting method is given as the iteration

$$(A^{\mathrm{T}}A + \alpha H_k)x_{k+1} = A^{\mathrm{T}}y, \tag{4.8}$$

where the matrix H_k is a discrete diffusion operator with the diffusion coefficient depending on the previous iterate x_k.

The next iterate x_{k+1} can be efficiently solved from (4.8) using the priorconditioned LSQR presented in Section 4.3 with H_k acting as the priorconditioner, see Publication IV. The reason for referring to H_k as priorconditioner instead of the standard term preconditioner arises from the nature of H_k. Typically, preconditioners are constructed from knowledge on the matrix that is being inverted. In this case, that matrix is $A^{\mathrm{T}}A$. However, H_k does not depend (directly) on $A^{\mathrm{T}}A$. Instead, H_k represents information about the expected solution. As the iteration (4.8) progresses, the features of the solution are progressively incorporated in the priorconditioner, allowing one to solve x_{k+1} from (4.8) with a low number of LSQR iterations.

5. Summary of results

Publication I extended the convex source support method to an unbounded domain in the framework of inverse source problems for the Poisson's equation and EIT. Specifically, the results of [23, 24] were adapted for the half-plane. The inverse source problem in a half-plane is significantly more ill-posed than that in the unit disc because the source, in a sense, masks itself more strongly in the former. In other words, the measurements are carried out only on one side of the unknown source. Nevertheless, the (appropriately modified) algorithm [23, 24] provides a good approximation for the discoidal source support.

Publication II introduced a novel two-electrode EIT measurement setting where one electrode resides at a fixed position while the other sweeps along the boundary of a two-dimensional domain. The difference data for this measurement configuration can be holomorphically continued to the complement of the support of an inclusion in an otherwise homogeneous domain. Consequently, the convex source support method is applicable to the sweep data. The performance of the corresponding algorithm was demonstrated using both an idealized point electrode model and the complete electrode model [12, 48].

Publication III extended the algorithm for computing the convex source support to a bounded three-dimensional domain. By substituting Kelvin transforms for Möbius transformations, the original discoidal domain of [23, 24] can be replaced by a ball. The new algorithm was tested in the frameworks of the inverse source problem for the Poisson's equation and EIT with a single current pattern.

Publication IV proposed the use of popular non-quadratic Tikhonov regularization penalties as preconditioners for solving ill-posed least-squares equations with Krylov subspace methods. In particular, a new variant of LSQR was derived, allowing efficient use of the proposed preconditioner. The performance of the method was demonstrated using a simple deblurring example and an inverse source problem for FDOT.

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